Electronic Supplementary Material (ESI) for ChemComm.

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Additional Figures

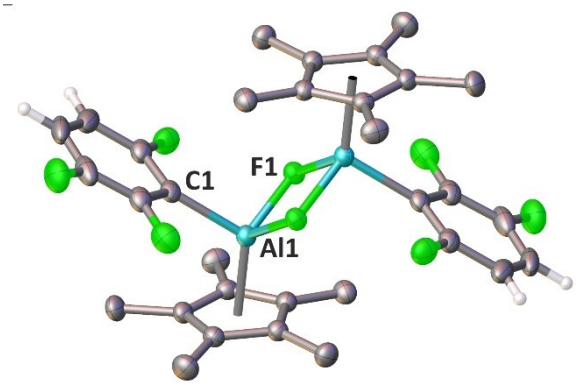

Figure S1. Solid-state structure of **4e** (hydrogen atoms except the aromatic protons are omitted for the sake of clarity). Selected bond lengths [Å] and angles [°] with calculated values (M06-2X/6-31G(d)//M06-2X(SMD)/6-311+G(d,p)) in square brackets: Al1–C1: 1.991(2) [1.981], Al1-F1 1.8452(14) [1.845], C1–Al1–F1 101.93(8) [100.19].

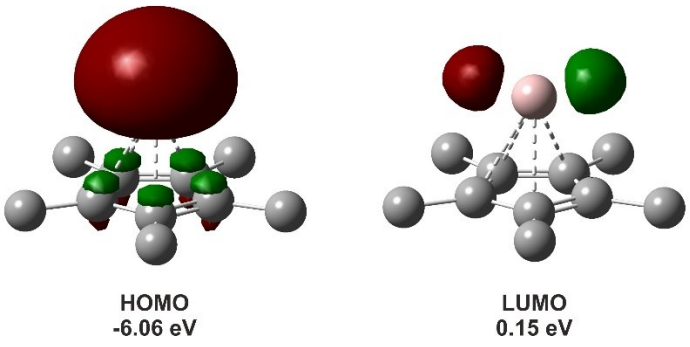

Figure S2. Representation and energies of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbital of **1'** as calculated at the M06-2X/6-31G(d)//M06-2X(SMD)/6-311+G(d,p) level of theory.

Experimental Procedures

General considerations

All preparations were performed under an inert atmosphere of dinitrogen by means of Standard Schlenk-line or glovebox (GS-Systemtechnik and MBraun) techniques. Toluene was used as p.a. grade and distilled from Na/benzophenone prior to use. C_6D_6 was dried over molecular sieves prior to use. Fluoroarenes were commercially available (Sigma Aldrich) and dried over molecular sieves prior to use. $(Cp^*Al)_4$ was prepared according to literature procedure.[1]

Characterization

The NMR spectra were recorded with Bruker Avance 400 and Bruker Fourier 300 spectrometers with δ referenced to external tetramethylsilane (^1H and ^{13}C) and CCl_3F (^{19}F). ^1H and ^{13}C NMR spectra were calibrated by using the solvent residual peak (C_6D_5H: $\delta(^1H)$ = 7.16) and the solvent peak (C_6D_6: $\delta(^{13}C)$ = 128.06), respectively. IR spectra (given in cm^{-1}) were recorded with an Agilent Cary 630 FT-IR spectrometer using a diamond ATR unit. Elemental analysis were conducted using a Vario EL Cube (Elementar-Analysensysteme), however, all samples were consistently low on carbon content, while providing satisfactory H and N values. Notably, elemental analysis of fluorine containing samples is sometimes complicated by the aggressive-ness of HF formed during the course of the combustion.

Synthetic procedures

Synthesis of {Cp(C_5F_4N)AlF}$_2$ (**4a**).* To a Schlenk vessel with 200 mg (1.23 mmol) of AlCp* in toluene (8 mL) 1 ml (9.11 mmol) of pentafluoropyridine C_5F_5N was added. The reaction mixture was stirred at room temperature for 1 week to achieve 80% conversion and 3 more hours at 90 ^oC to complete a reaction. Obtained solution was filtrated, concentrated and the product was crystallized at -30 ^oC. **4a** was isolated as colourless crystals in the amount of 127 mg (31 % yield). ^1H NMR (400 MHz, C_6D_6): δ = 1.37 (s, 30H, $C_5\mathit{Me_5}$); $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 9.4 ($C_5\mathit{Me_5}$), 114.5 ($\mathit{C_5}Me_5$), the remaining carbon atoms of the C_5F_4N substituent are not resolved due to multiple coupling to ^{19}F and line broadening by ^{27}Al; ^{19}F NMR (377 MHz, C_6D_6): δ = -93.75 (m, C-*F*), -109.20 (s, broad, Al-*F*), -124.50 (m, C-*F*); ATR-IR: 691, 920, 1163, 1209, 1364, 1384, 1414, 1429, 1451, 1627, 2868, 2918, 2961; Elemental analysis found (calc) $C_{30}H_{30}Al_2F_{10}N_2$: C 53.32 (54.38), H 4.65 (4.53); N 4.03 (4.23).

Synthesis of {Cp(C_7F_7)AlF}$_2$ (**4b**).* To a Schlenk vessel with 200 mg (1.23 mmol) of AlCp* in toluene (10 mL) 1 ml (7,08 mmol) of octafluorotoluene was added. The reaction mixture was stirred on heating at 90 ^oC for 15 minutes to obtain clear colourless solution. The solution was concentrated and the product was crystallized at -30 ^oC. **4b** was isolated as colourless crystals in the amount of 278 mg (57 % yield). ^1H NMR (400 MHz, C_6D_6): δ = 1.40 (s, 30 H, $C_5\mathit{Me_5}$), 1.65 (s, 7.5 H, $C_5\mathit{Me_5}$); $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 9.4 ($C_5\mathit{Me_5}$), 10.1 (weak, $C_5\mathit{Me_5}$), 114.4 ($\mathit{C_5}Me_5$), 115.2 (weak, $\mathit{C_5}Me_5$), the remaining carbon atoms of the C_7F_7 substituent are not resolved due to multiple coupling to ^{19}F and line broadening by ^{27}Al; ^{19}F NMR (377 MHz, C_6D_6): δ = -56.05 (t, J_{FF} = 23 Hz, CF_3), -56.60 (weak, t, J_{FF} = 23 Hz, CF_3), -109.20 (s, broad, Al-*F*), -118.85 (m, C-*F* aromatic), -119.61 (weak, m, C-*F* aromatic), -140.46 (m, C-*F* aromatic), -140.90 (weak, m, C-*F* aromatic); ATR-IR: 712, 920, 951, 1072, 1115, 1133, 1180, 1316, 1383, 1439, 1584, 1648, 2042, 2164, 2870, 2920, 2963; Elemental analysis found (calc) $C_{34}H_{30}Al_2F_{16}$: C 50.65 (51.26), H 4.26 (3.77).

Synthesis of {Cp(C_6F_5)AlF}$_2$ (**4c**).* To a Schlenk vessel with 200 mg (1.23 mmol) of AlCp* in toluene (8 mL) 1 ml (8.66 mmol) of hexafluorobenzene C_6F_6 was added. The reaction mixture was stirred on heating at 90 ^oC for 24 hours. Obtained solution was filtrated, concentrated and the product was crystallized at -30 ^oC. **4c** was isolated as colourless crystals in the amount of 110 mg (26 % yield). ^1H NMR (400 MHz, C_6D_6): δ = 1.46 (s, 30H, C_5*Me$_5$*); $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 9.5 (C_5*Me$_5$*), 114.3 (*C$_5$*Me$_5$), the remaining carbon atoms of the C_6F_5 substituent are not resolved due to multiple coupling to ^{19}F and line broadening by ^{27}Al; ^{19}F NMR (377 MHz, C_6D_6): δ = -109.85 (s, broad, Al-*F*), -120.04 (d, $^3J_{FF}$ = 19 Hz, C-*F* in *o*-position to Al), -120.54 (weak, m, C-*F*), -153.56 (t, $^3J_{FF}$ = 19 Hz, C-*F* in *p*-position to Al), -154.67 (weak, m, C-*F*), -161.09 (m, C-*F* in *m*-position to Al), -161.75 (weak, m, C-*F*); ATR-IR: 721, 924, 956, 1025, 1060, 1069, 1271, 1360, 1379, 1442, 1508, 1636, 2864, 2916, 2954; Elemental analysis found (calc) $C_{32}H_{30}Al_2F_{12}$: C 51.39 (55.18), H 4.35 (4.31).

Synthesis of {Cp(C_6HF_4)AlF}$_2$ (**4d**).* To a Schlenk vessel with 200 mg (1.23 mmol) of AlCp* in toluene (10 mL) 1 ml (8.99 mmol) of pentafluorobenzene C_6F_5H was added. The reaction mixture was stirred on heating at 90 ^oC for 24 hours. Obtained solution was concentrated and the product was crystallized at -30 ^oC. **4d** was isolated as colourless crystals in the amount of 169 mg (42 % yield). ^1H NMR (400 MHz, C_6D_6): δ = 1.54 (s, 30H, C_5*Me$_5$*), 6.50 (m, 2H, C-*H* aromatic); $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 9.6 (C_5*Me$_5$*), 106.1 (t, $^2J_{CF}$ = 23 Hz, *C*-H aromatic), 114.3 (*C$_5$*Me$_5$), the remaining carbon atoms of the C_6HF_4 substituent are not resolved due to multiple coupling to ^{19}F and line broadening by ^{27}Al; ^{19}F NMR (377 MHz, C_6D_6): δ = -109.66 (s, broad, Al-*F*), -121.43 (m, C-*F*), -139.01 (m, C-*F*); ATR-IR: 705, 850, 960, 1137, 1163, 1204, 1344, 1377, 1441, 1590, 2866, 2924, 2986; Elemental analysis found (calc) $C_{32}H_{32}Al_2F_{10}$: C 55.72 (58.19), H 4.88 (4.88).

Synthesis of {Cp($C_6H_2F_3$)AlF}$_2$ (**4e**).* To a Schlenk vessel with 200 mg (1.23 mmol) of AlCp* in toluene (10 mL) 1 ml (6.9 mmol) of 1,2,3,4-tetrafluorobenzene $C_6F_4H_2$ was added. The reaction mixture was stirred on heating at 90 ^oC for 5 days. Obtained solution was concentrated and the product was crystallized at -30 ^oC. **4e** was isolated as colourless crystals in the amount of 87 mg (23 % yield). ^1H NMR (400 MHz, C_6D_6): δ = 1.63 (s, 30H, C_5*Me$_5$*), 6.41 (m, 2H, C-*H* aromatic), 6.62 (m, 2H, C-*H* aromatic); $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 9.7 (C_5*Me$_5$*), 110.6 (d, $^2J_{CF}$ = 15 Hz, *C*-H aromatic), 114.3 (*C$_5$*Me$_5$), 117.3 (m, *C*-H aromatic), the remaining carbon atoms of the C_6HF_4 substituent are not resolved due to multiple coupling to ^{19}F and line broadening by ^{27}Al; ^{19}F NMR (377 MHz, C_6D_6): δ = -96.93 (m, C-*F*), -109.85 (s, broad, Al-*F*), -115.38 (m, C-*F*), -144.29 (m, C-*F*); ATR-IR: 721, 731, 809, 854, 960, 978, 1165, 1219, 1383, 1407, 1450, 1582, 1616, 2865, 2917, 2980; Elemental analysis found (calc) $C_{32}H_{34}Al_2F_8$: C 58.64 (61.54), H 5.44 (5.49).

Crystallographic details

The intensity data for the compounds were collected on a Nonius KappaCCD diffractometer using graphite-monochromated Mo-K_α radiation. Data were corrected for Lorentz and polarization effects; absorption was taken into account on a semi-empirical basis using multiple-scans.[2-4] The structures were solved by direct methods (SHELXS)[5] and refined by full-matrix least squares techniques against Fo^2 (SHELXL-2018).[6] All hydrogen atoms were included at calculated positions with fixed thermal parameters. All non-hydrogen atoms were refined anisotropically.[6] Crystallographic data as well as structure solution and refinement details are summarized in Table S1. Olex2[7] was used for structure representations.

Crystallographic data (excluding structure factors) has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC-1971668 for **4a**, CCDC-1971669 for **4b**, CCDC-1971670 for **4c**, CCDC-1971671 for **4d**, and CCDC-1971672 for **4e**. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [E- mail: deposit@ccdc.cam.ac.uk].

Table S1. Crystal data and refinement details for the X-ray structure determinations.

Compound	**4a**	**4b**	**4c**	**4d**	**4e**
formula	$C_{30}H_{30}Al_2F_{10}N_2$	$C_{34}H_{30}Al_2F_{16}$	$C_{32}H_{30}Al_2F_{12}$	$C_{32}H_{32}Al_2F_{10}$	$C_{32}H_{34}Al_2F_8$
fw ($g \cdot mol^{-1}$)	662.52	796.54	696.52	660.53	624.55
T/°C	-140(2)	-140(2)	-140(2)	-140(2)	-140(2)
crystal system	triclinic	triclinic	monoclinic	monoclinic	monoclinic
space group	P $\bar{1}$	P $\bar{1}$	C 2/c	P 2_1/n	P 2_1/n
a/ Å	8.4228(2)	8.4379(2)	17.0235(4)	9.1602(2)	9.1825(4)
b/ Å	9.8609(3)	9.9671(3)	10.2649(2)	21.9370(7)	10.7930(5)
c/ Å	10.1038(4)	11.3803(3)	17.3300(4)	14.8657(5)	14.8825(7)
α/°	65.090(1)	115.809(1)	90	90	90
β/°	72.958(2)	98.981(2)	94.820(1)	97.288(2)	99.315(3)
γ/°	85.464(2)	92.895(1)	90	90	90
V/Å^3	726.74(4)	843.48(4)	3017.61(12)	2963.09(15)	1455.51(12)
Z	1	1	4	4	2
ρ ($g \cdot cm^{-3}$)	1.514	1.568	1.533	1.481	1.425
μ (cm^{-1})	1.89	2.01	1.94	1.84	1.73
measured data	5879	11683	8935	21742	16706
data with I > 2σ(I)	3002	3365	2856	4481	2837
unique data (R_{int})	3253/0.0201	3838/0.0243	3447/0.0381	6764/0.1197	3318/0.0661
wR_2 (all data, on F^2)[a]	0.0888	0.0978	0.1025	0.1414	0.1332
R_1 ($I > 2\sigma(I)$) [a]	0.0355	0.0393	0.0468	0.0764	0.0582
S [b]	1.064	1.037	1.067	1.063	1.089
Res. dens./$e \cdot Å^{-3}$	0.357/-0.228	0.356/-0.201	0.334/-0.261	0.380/-0.422	0.342/-0.359
absorpt method	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
absorpt corr $T_{min}/_{max}$	0.7261/0.7456	0.7058/0.7456	0.6971/0.7456	0.6505/0.7456	0.5539/0.7455
CCDC No.	1971668	1971669	1971670	1971671	1971672

[a] Definition of the *R* indices: $R_1 = (\Sigma \,||F_o| - |F_c||)/\Sigma |F_o|$;
$wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ with $w^{-1} = \sigma^2(F_o^2) + (aP)^2+bP$; $P = [2F_c^2 + \mathrm{Max}(F_O^2]/3$;
[b] $s = \{\Sigma[w(F_o^2-F_c^2)^2]/(N_o-N_p)\}^{1/2}$.

NMR and IR spectra

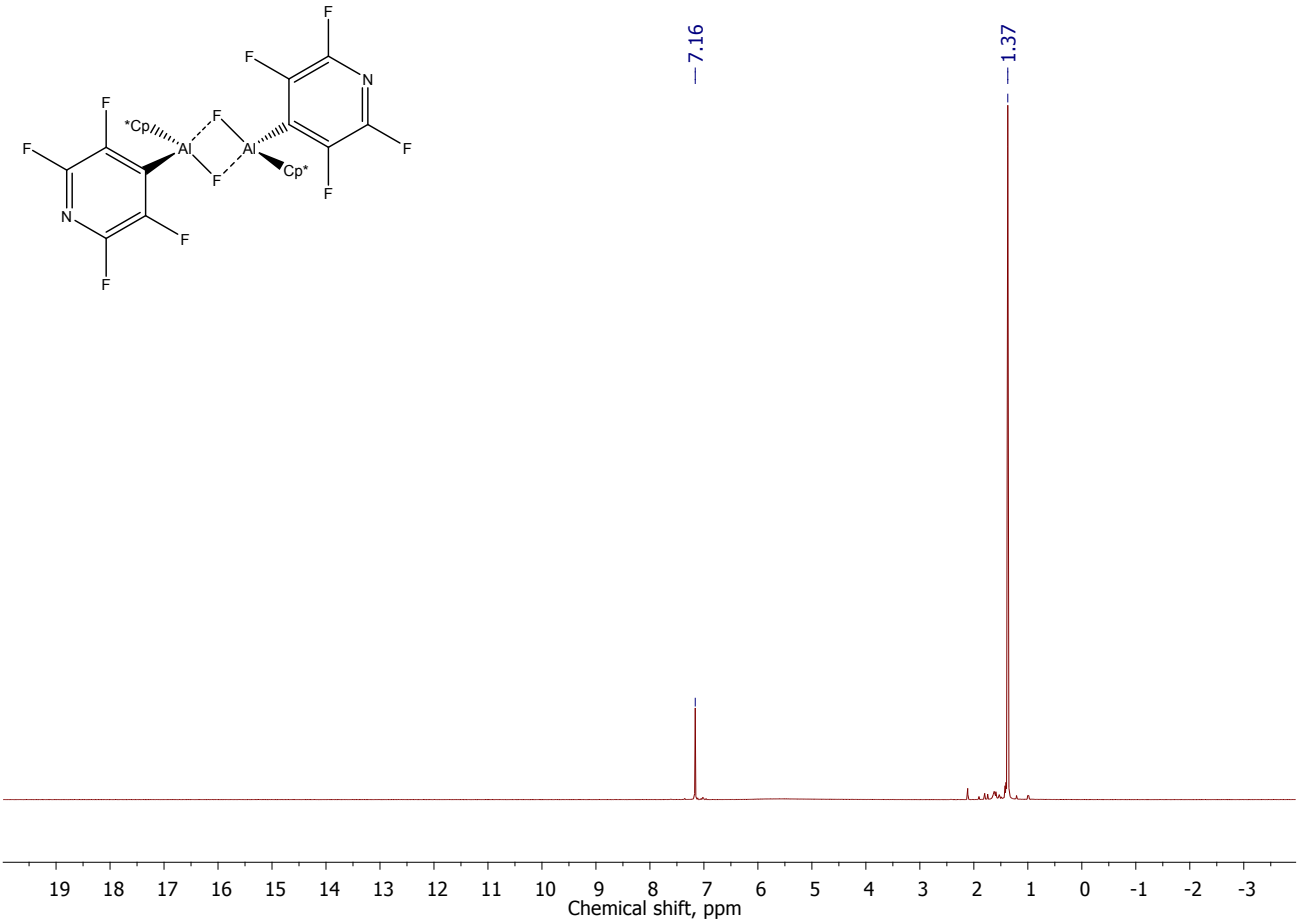

Figure S3. ^{1}H NMR spectrum (400 MHz) of {Cp*(C_5F_4N)AlF}$_2$ (**4a**) in C_6D_6 (peak of solvent at 7.16 ppm).

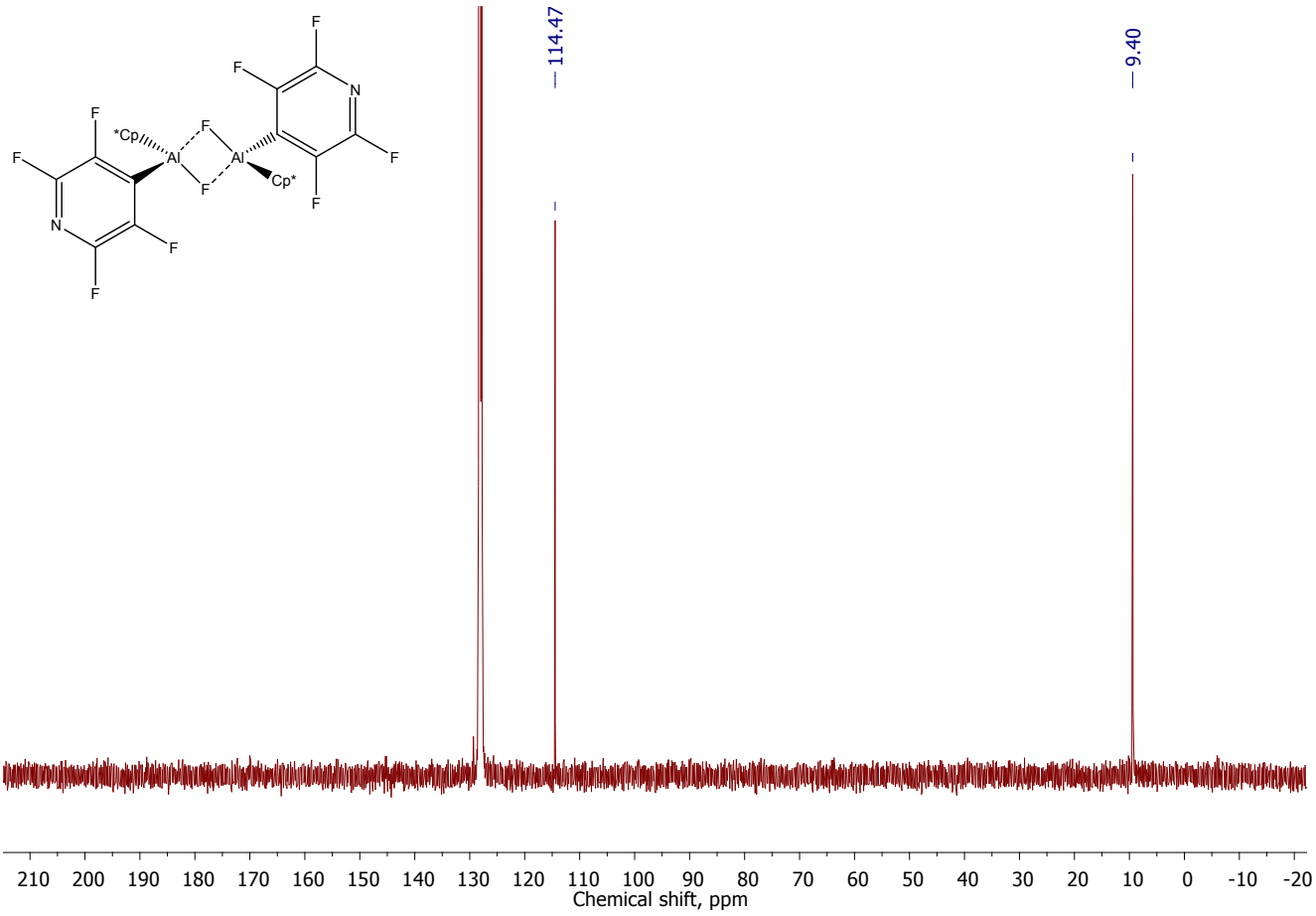

Figure S4. ^{13}C NMR spectrum (101 MHz) of $\{Cp^*(C_5F_4N)AlF\}_2$ (**4a**) in C_6D_6 (peak of solvent at 128 ppm).

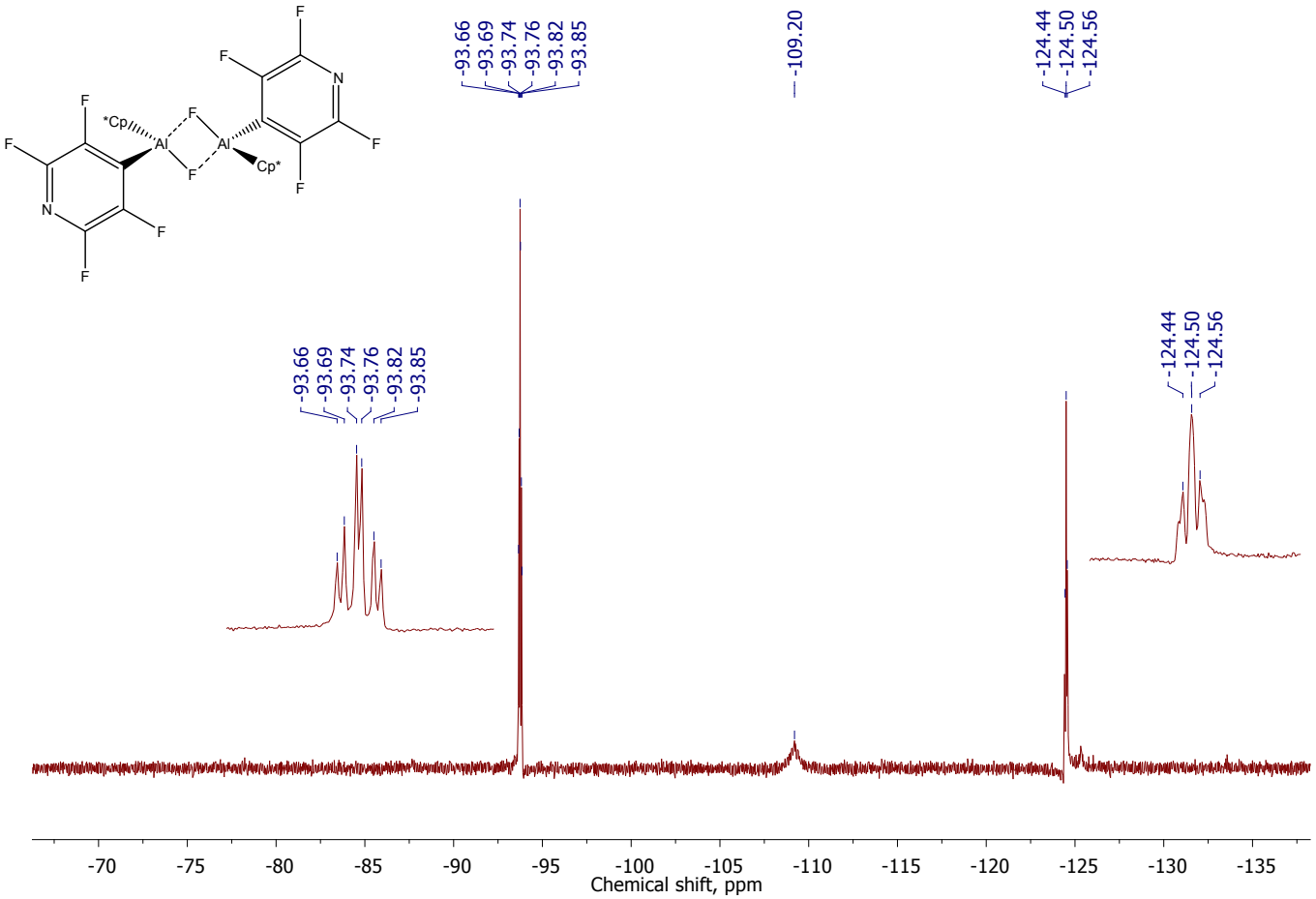

Figure S5. ^{19}F NMR spectrum (377 MHz) of $\{Cp^*(C_5F_4N)AlF\}_2$ (**4a**) in C_6D_6 and its magnified sections.

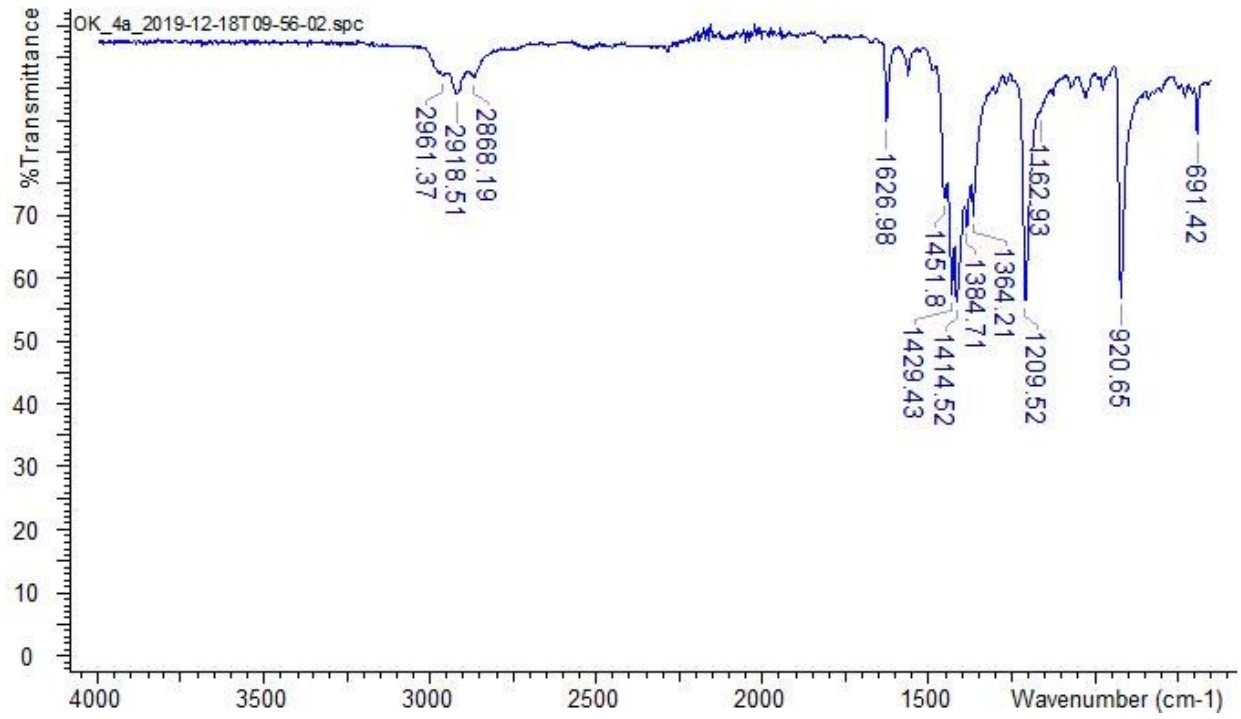

Figure S6. ATR-IR spectrum (diamond) of $\{Cp^*(C_5F_4N)AlF\}_2$ (**4a**).

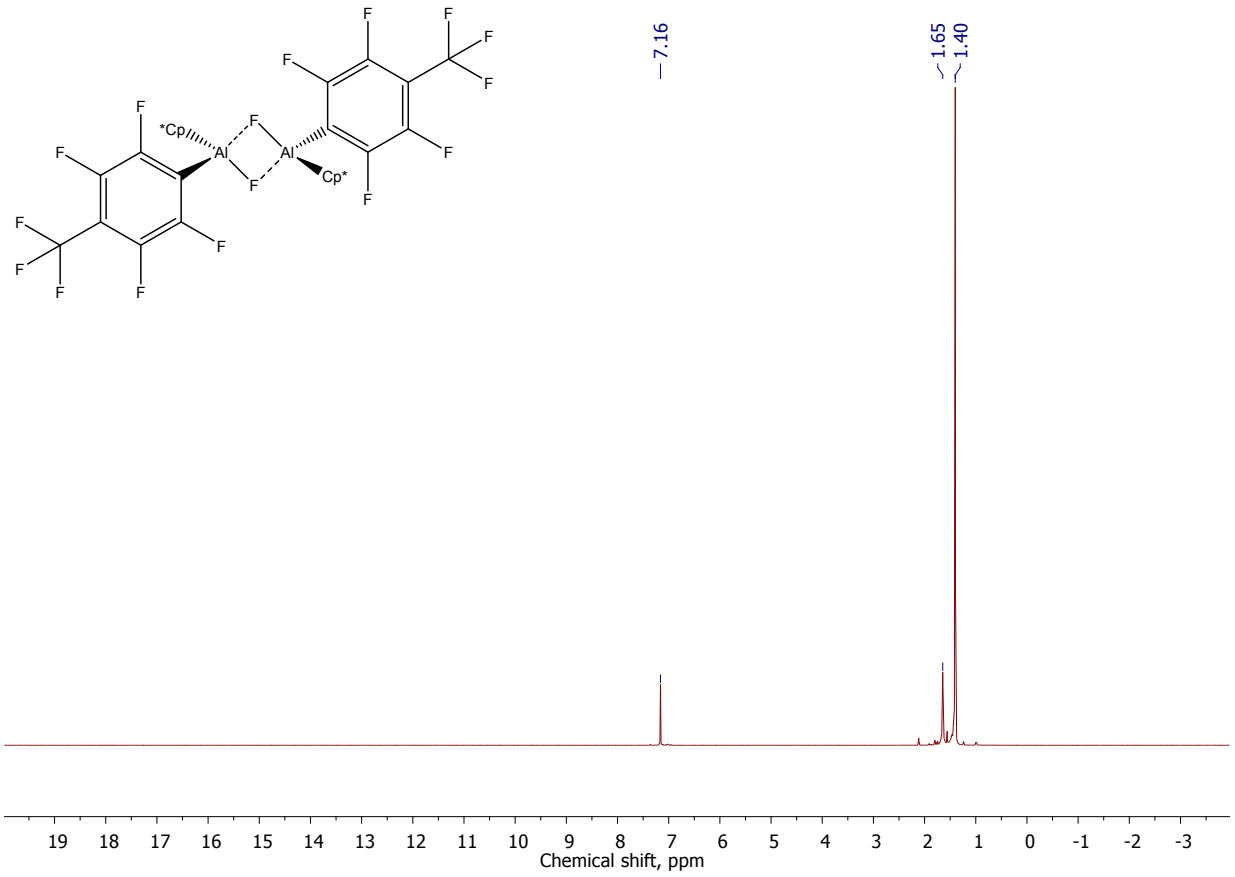

Figure S7. ^{1}H NMR spectrum (400 MHz) of {Cp*(C_7F_7)AlF}$_2$ (**4b**) in C_6D_6 (peak of solvent at 7.16 ppm).

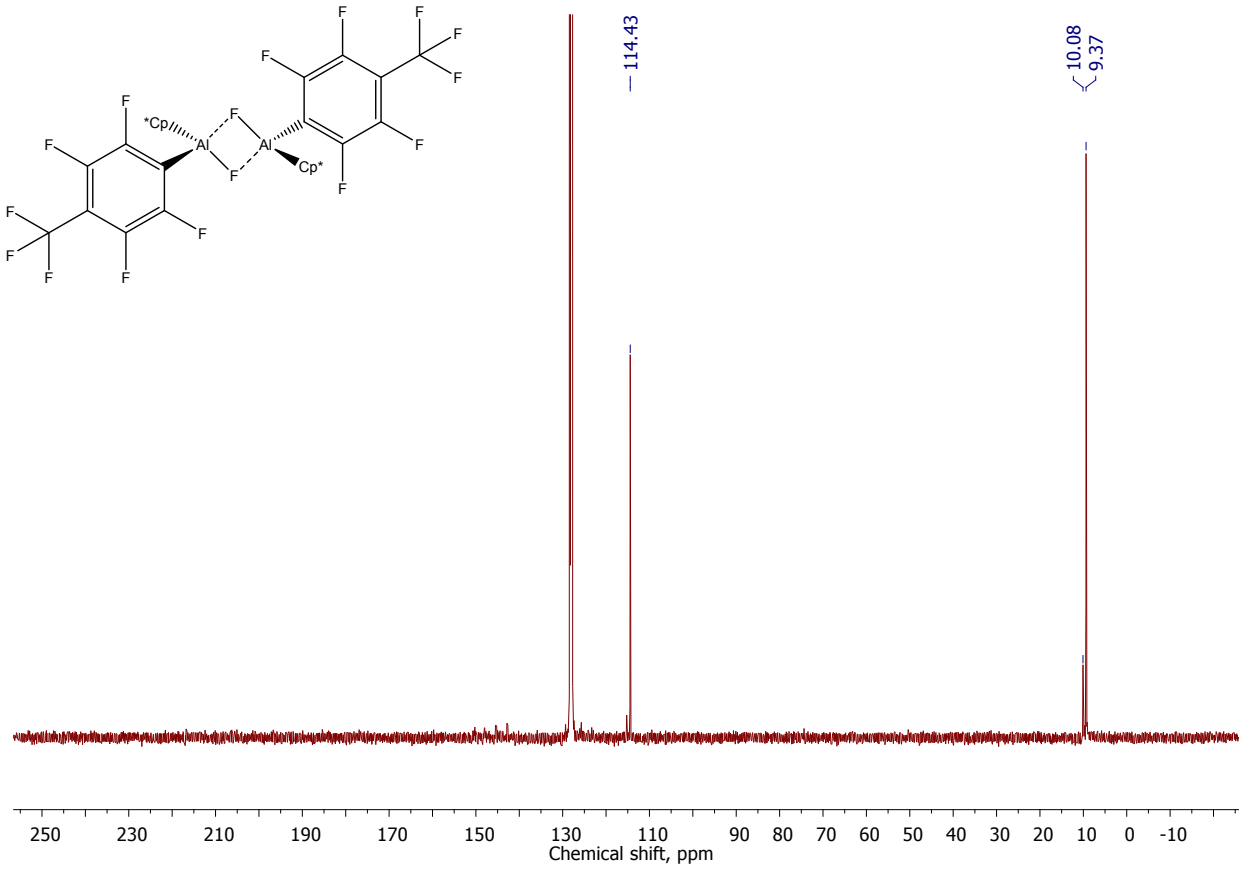

Figure S8. ^{13}C NMR spectrum (101 MHz) of $\{Cp^*(C_7F_7)AlF\}_2$ (**4b**) in C_6D_6 (peak of solvent at 128 ppm).

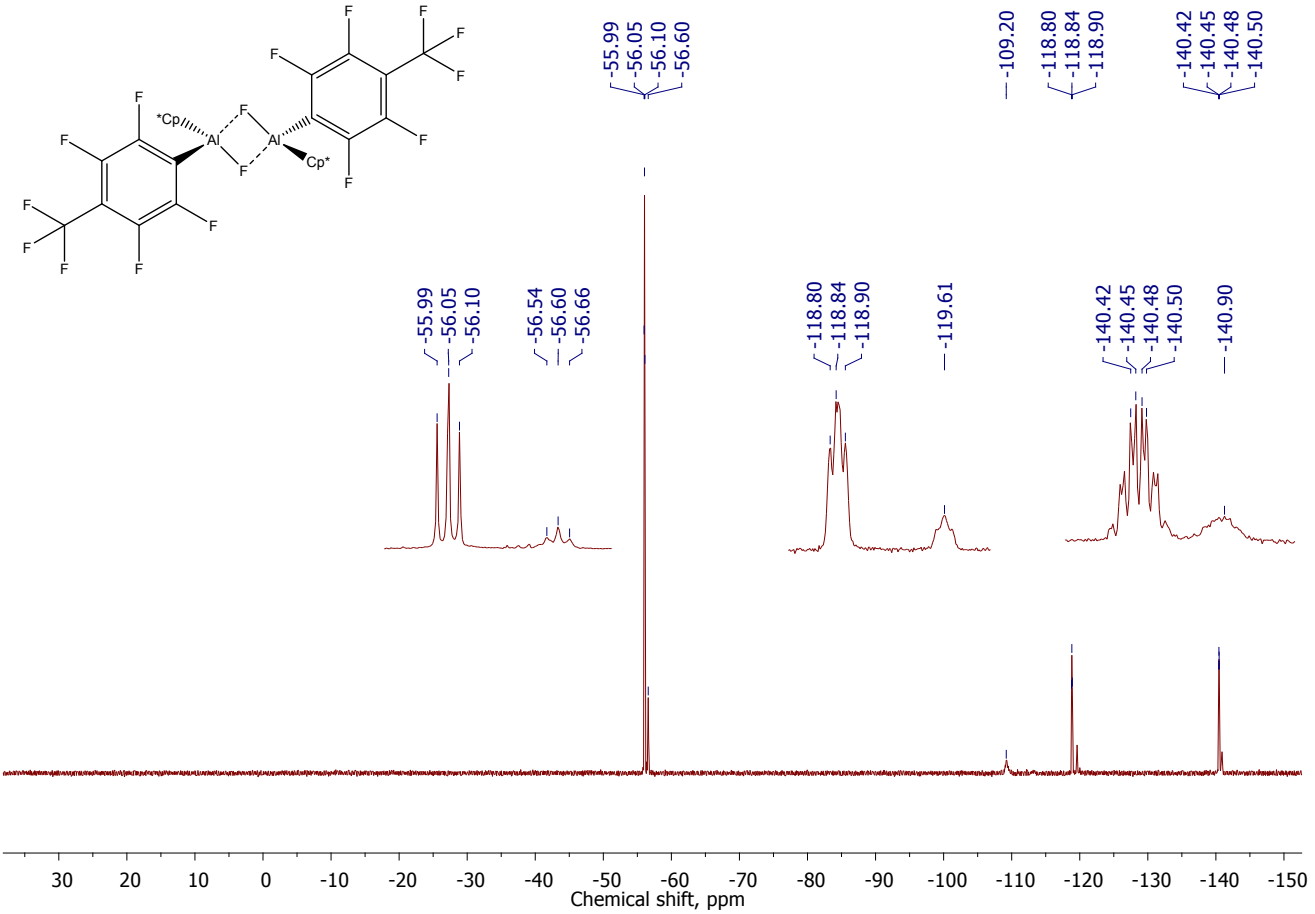

Figure S9. ^{19}F NMR spectrum (377 MHz) of $\{Cp^*(C_7F_7)AlF\}_2$ (**4b**) in C_6D_6 and its magnified sections.

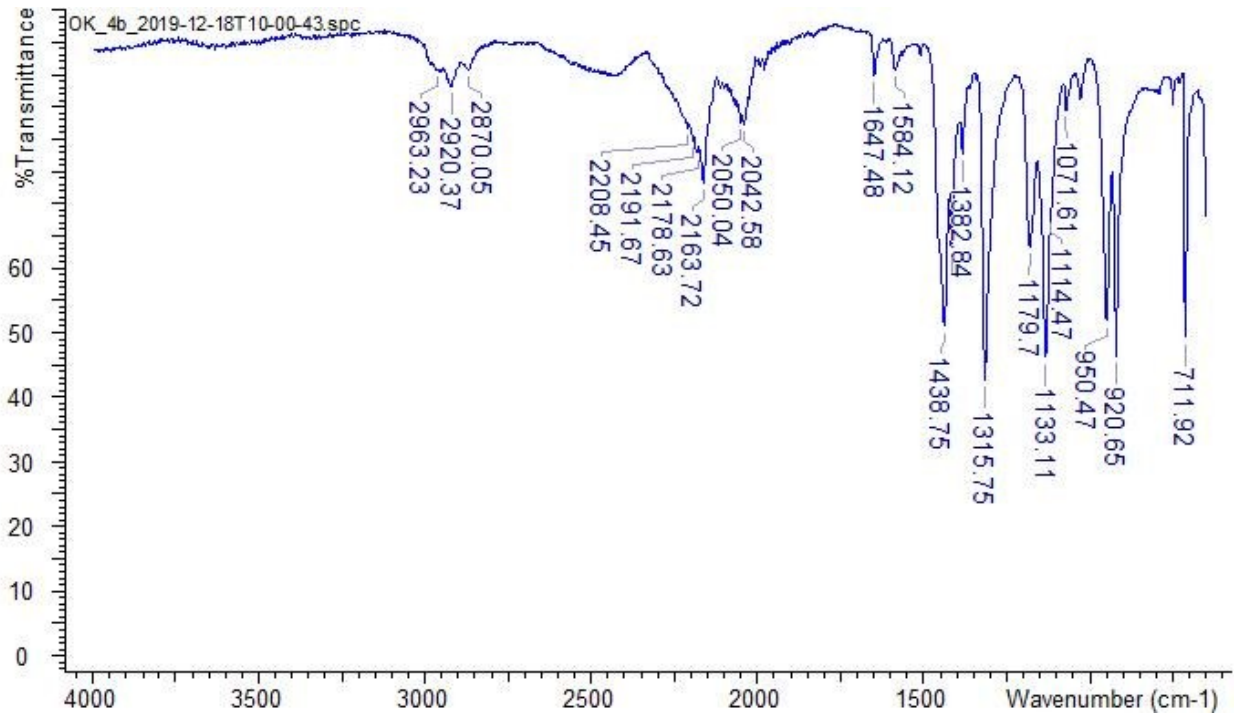

Figure S10. ATR-IR spectrum (diamond) of $\{Cp^*(C_7F_7)AlF\}_2$ (**4b**).

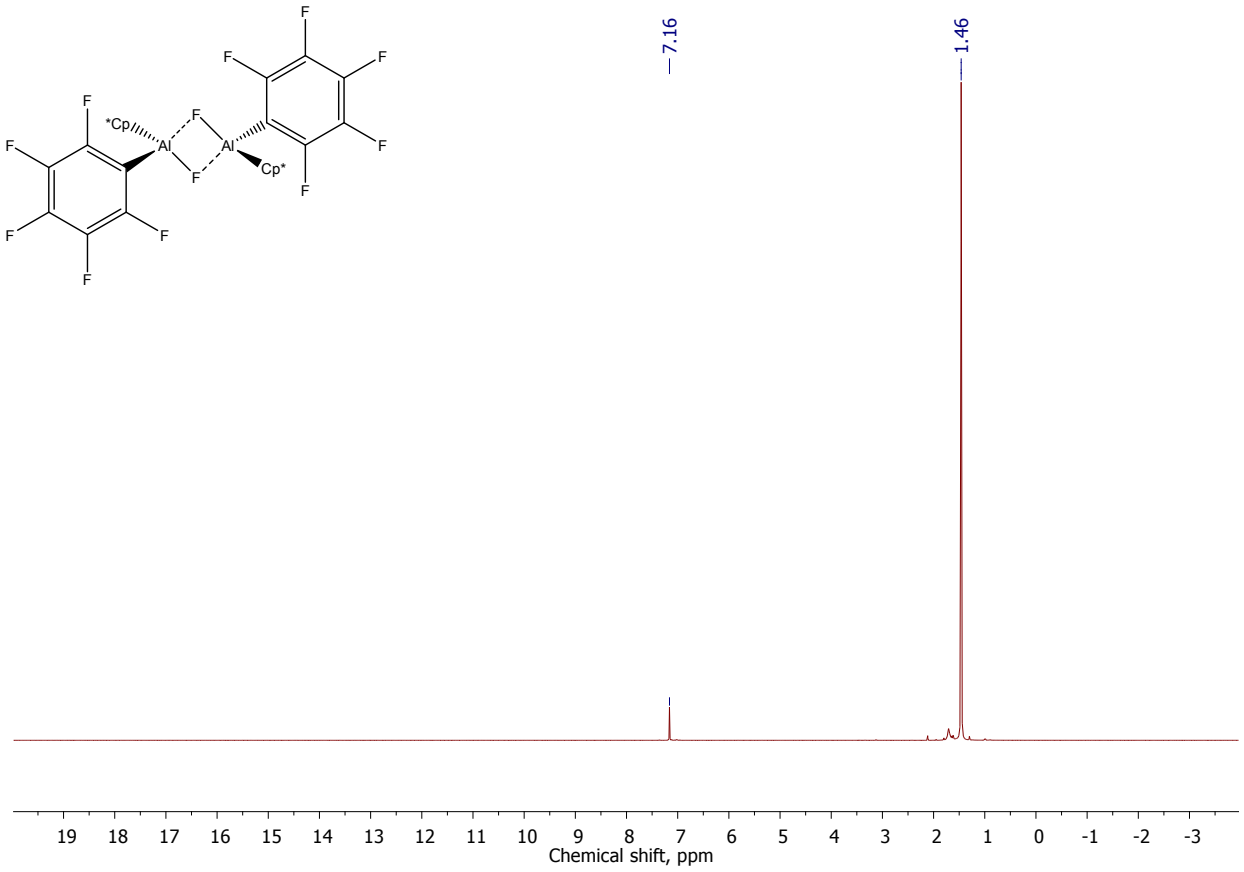

Figure S11. ^{1}H NMR spectrum (400 MHz) of $\{Cp^*(C_6F_5)AlF\}_2$ (**4c**) in C_6D_6 (peak of solvent at 7.16 ppm).

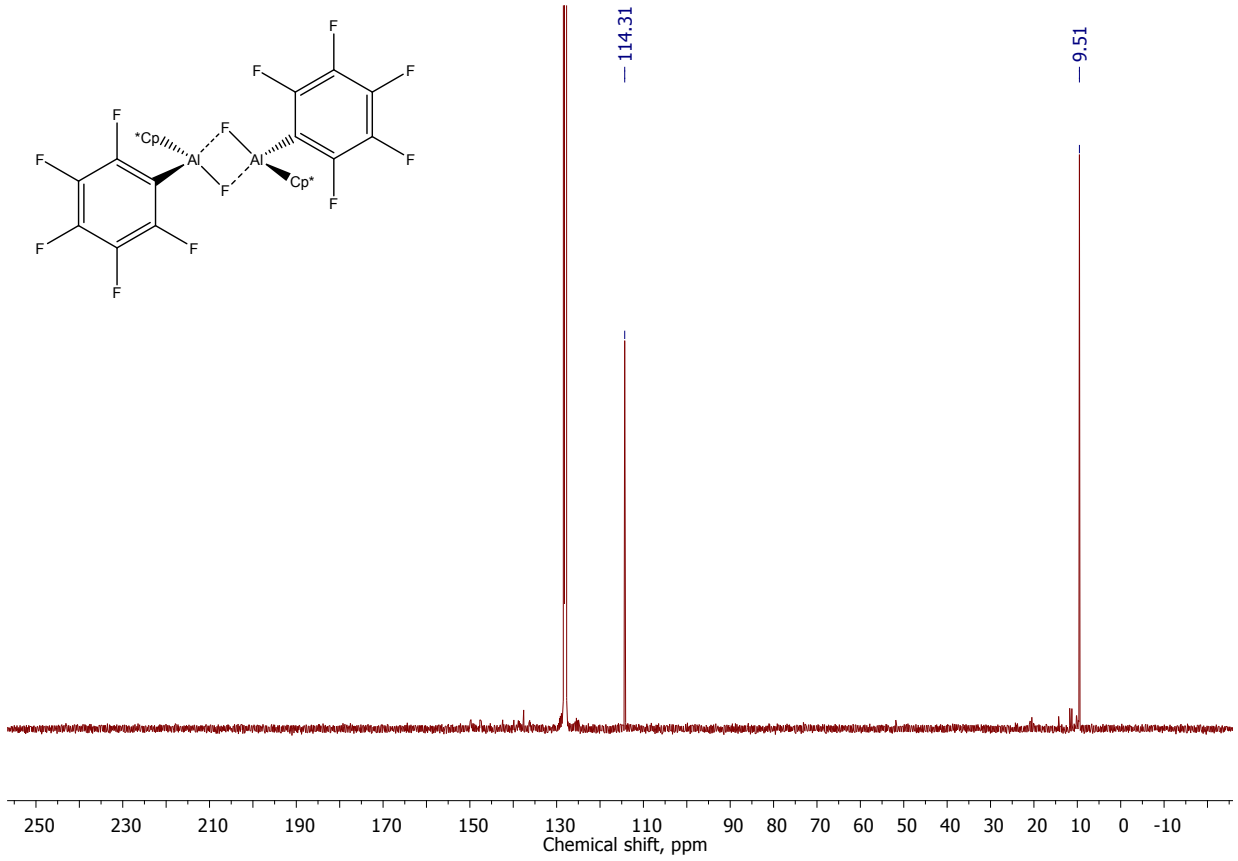

Figure S12. ^{13}C NMR spectrum (101 MHz) of $\{Cp^*(C_6F_5)AlF\}_2$ (**4c**) in C_6D_6 (peak of solvent at 128 ppm).

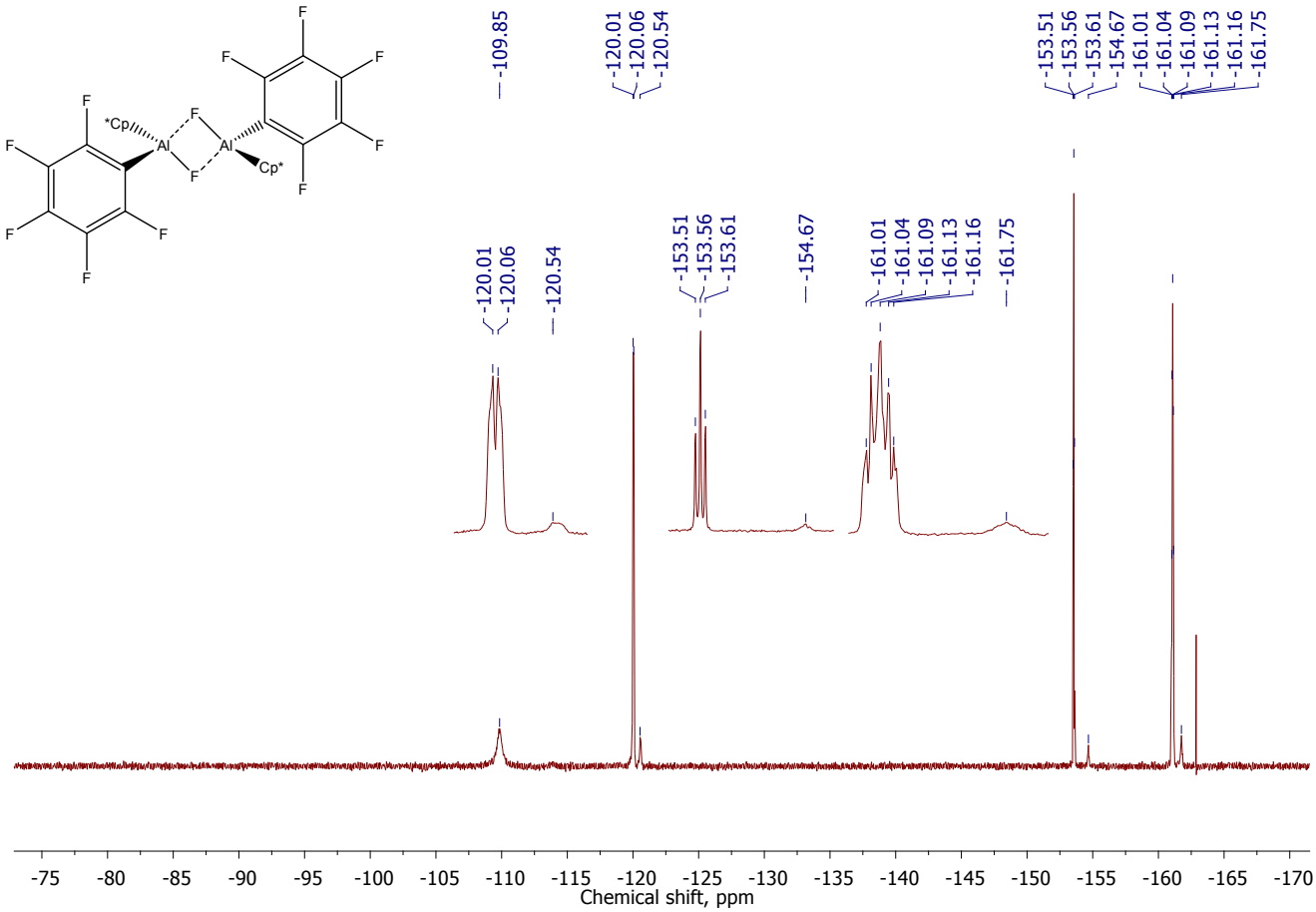

Figure S13. ^{19}F NMR spectrum (377 MHz) of $\{Cp^*(C_6F_5)AlF\}_2$ (**4c**) in C_6D_6 and its magnified sections.

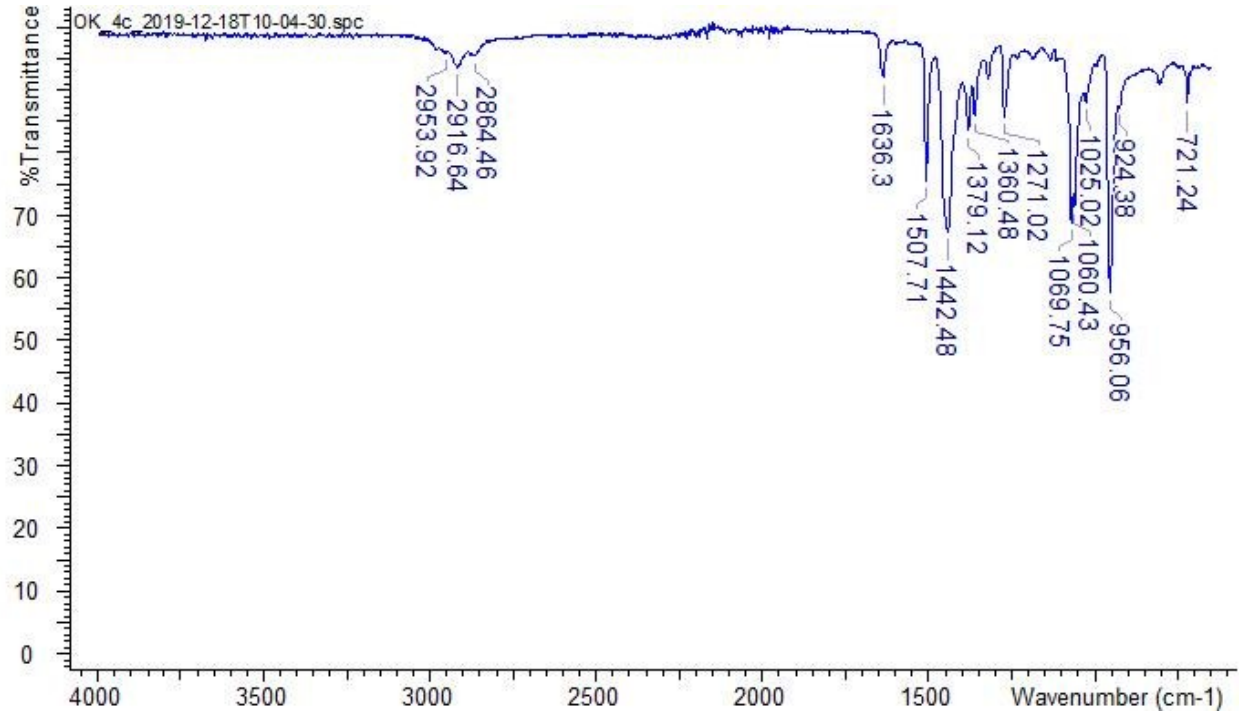

Figure S14. ATR-IR spectrum (diamond) of $\{Cp^*(C_6F_5)AlF\}_2$ (**4c**).

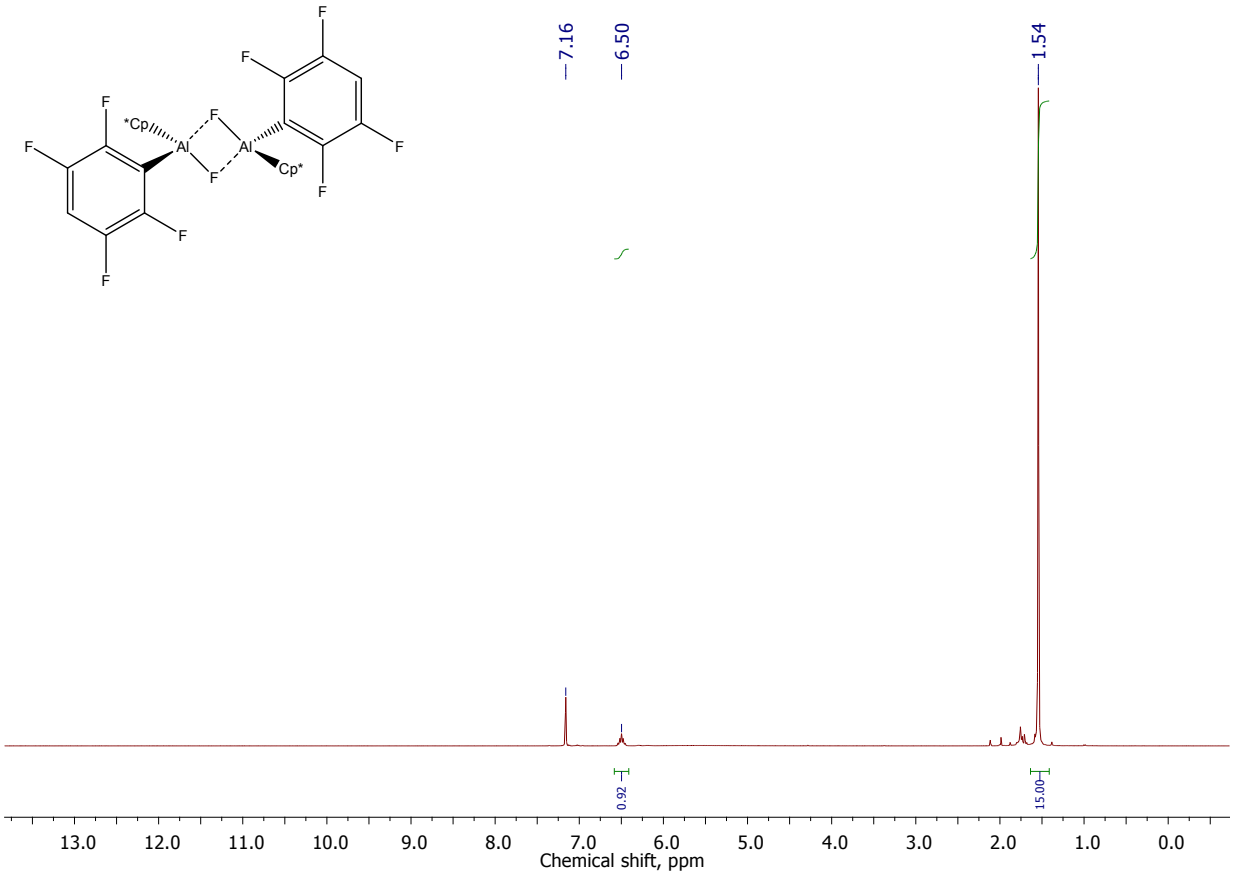

Figure S15. ^{1}H NMR spectrum (400 MHz) of {Cp*(C_6F_4H)AlF}$_2$ (**4d**) in C_6D_6 (peak of solvent at 7.16 ppm).

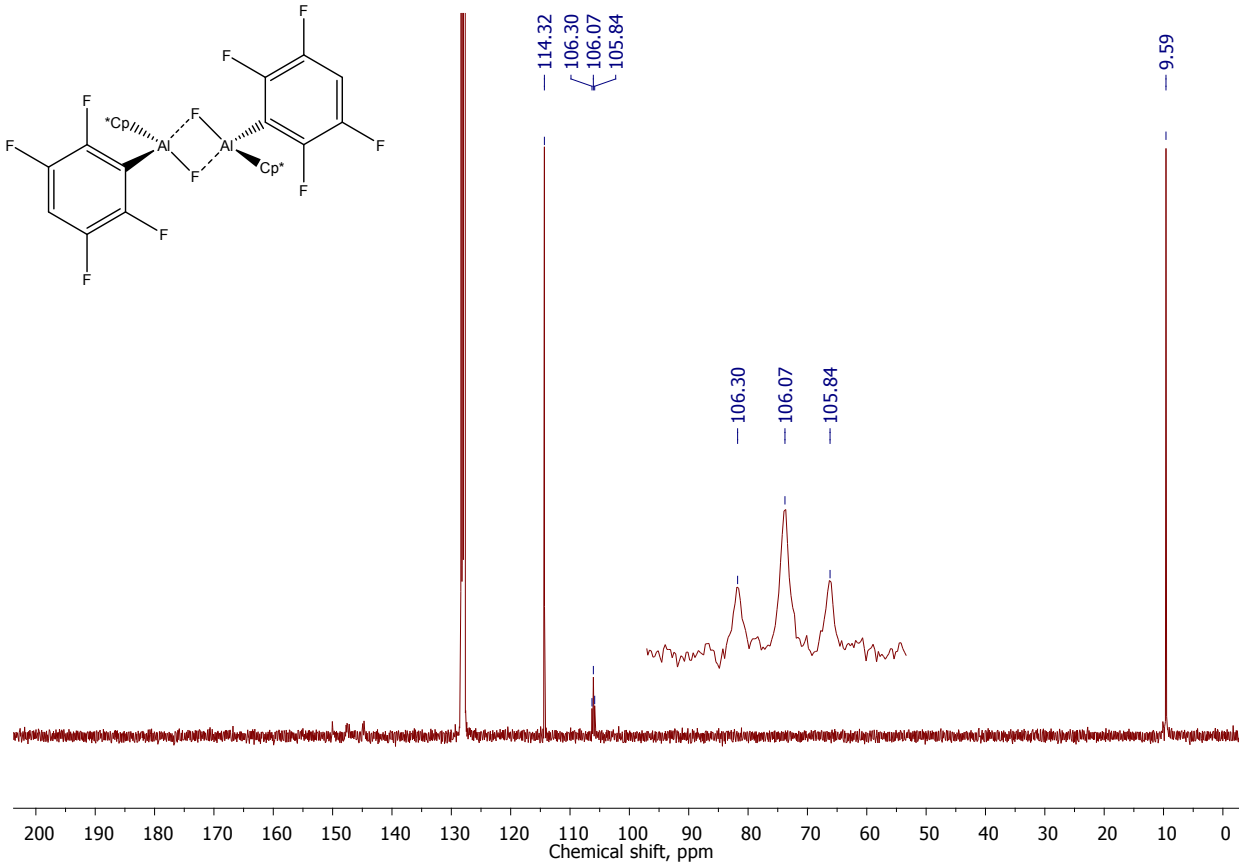

Figure S16. ^{13}C NMR spectrum (101 MHz) of $\{Cp^*(C_6F_4H)AlF\}_2$ (**4d**) in C_6D_6 (peak of solvent at 128 ppm) and its magnified section.

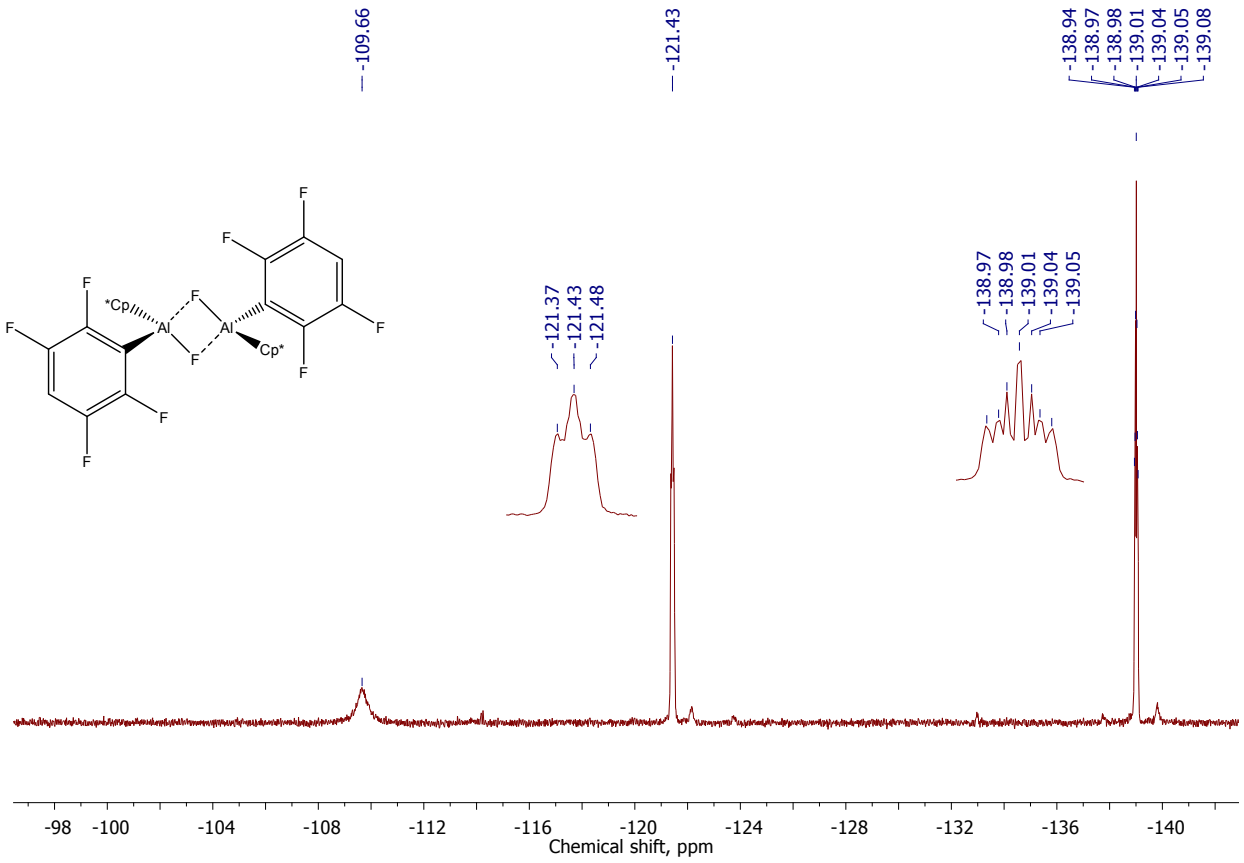

Figure S17. ^{19}F NMR spectrum (377 MHz) of $\{Cp^*(C_6F_4H)AlF\}_2$ (**4d**) in C_6D_6 and its magnified sections.

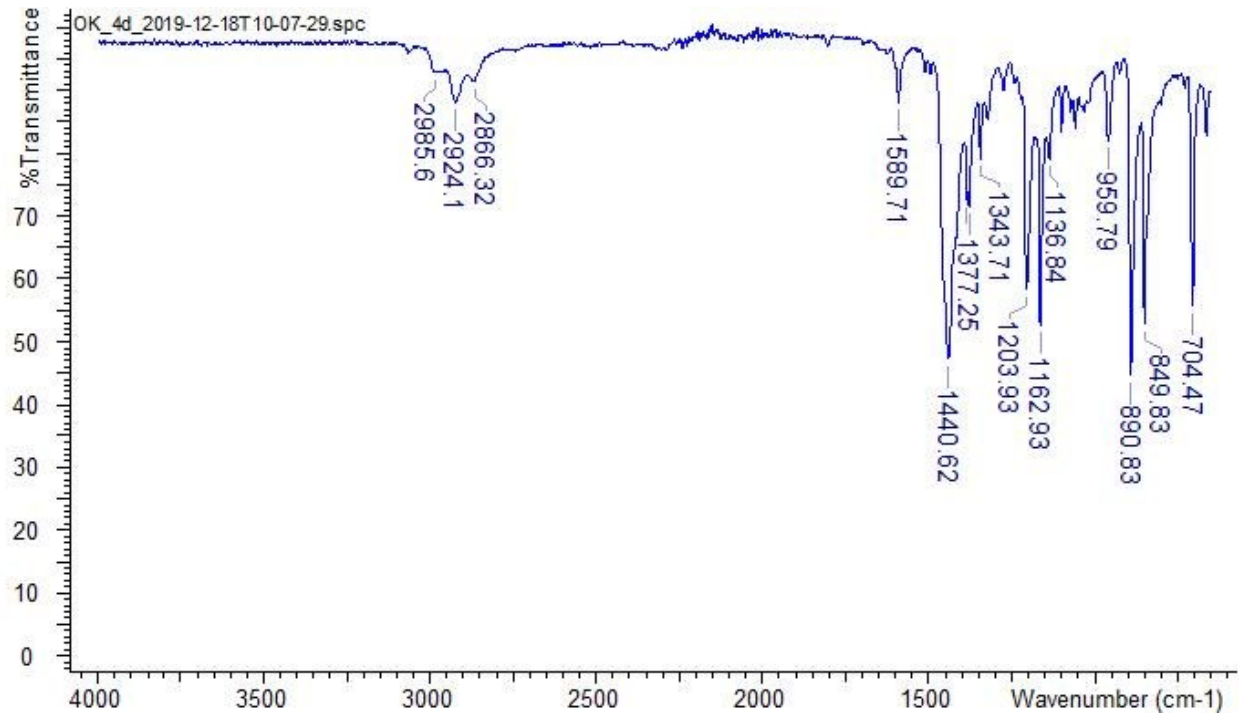

Figure S18. ATR-IR spectrum (diamond) of $\{Cp^*(C_6F_4H)AlF\}_2$ (**4d**).

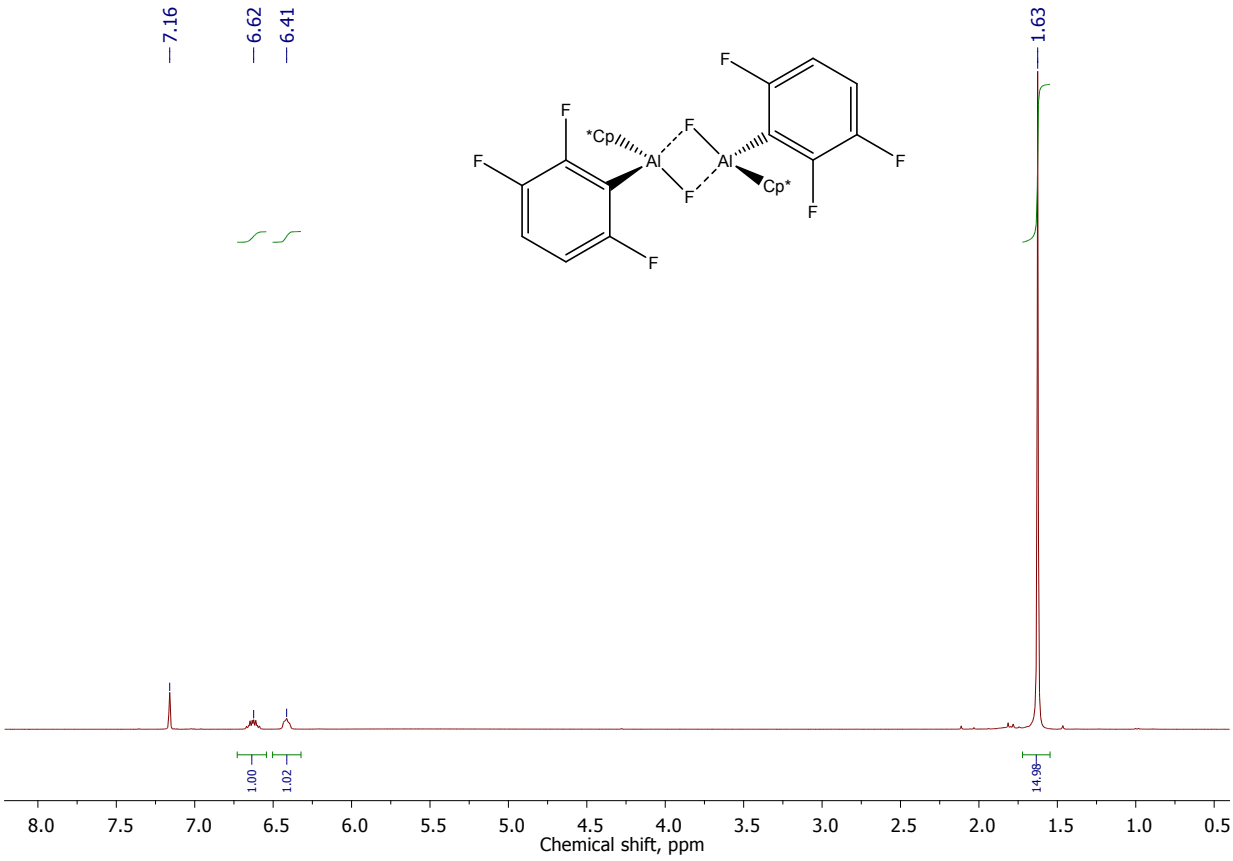

Figure S19. ^{1}H NMR spectrum (400 MHz) of $\{Cp^*(C_6F_3H_2)AlF\}_2$ (**4e**) in C_6D_6 (peak of solvent at 7.16 ppm).

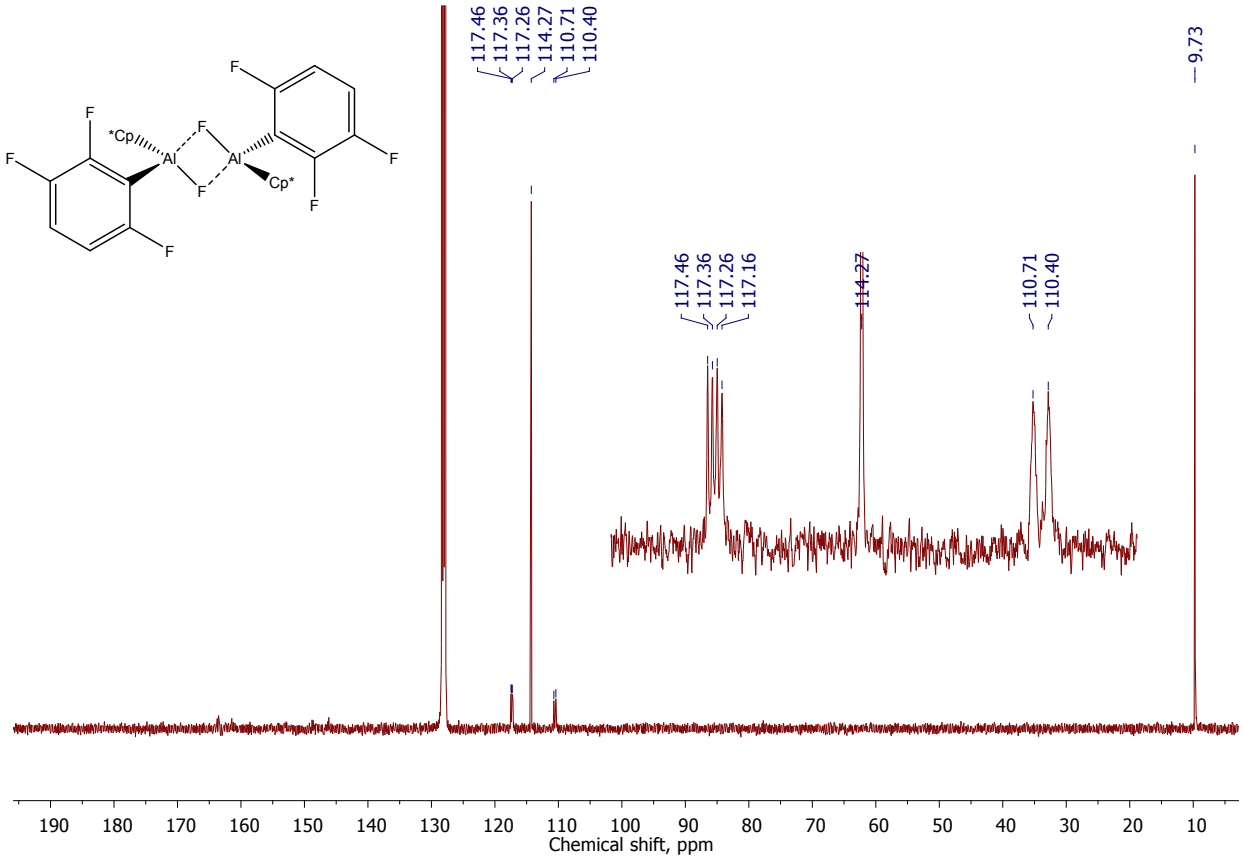

Figure S20. ^{13}C NMR spectrum (101 MHz) of $\{Cp^*(C_6F_3H_2)AlF\}_2$ (**4e**) in C_6D_6 (peak of solvent at 128 ppm) and its magnified section.

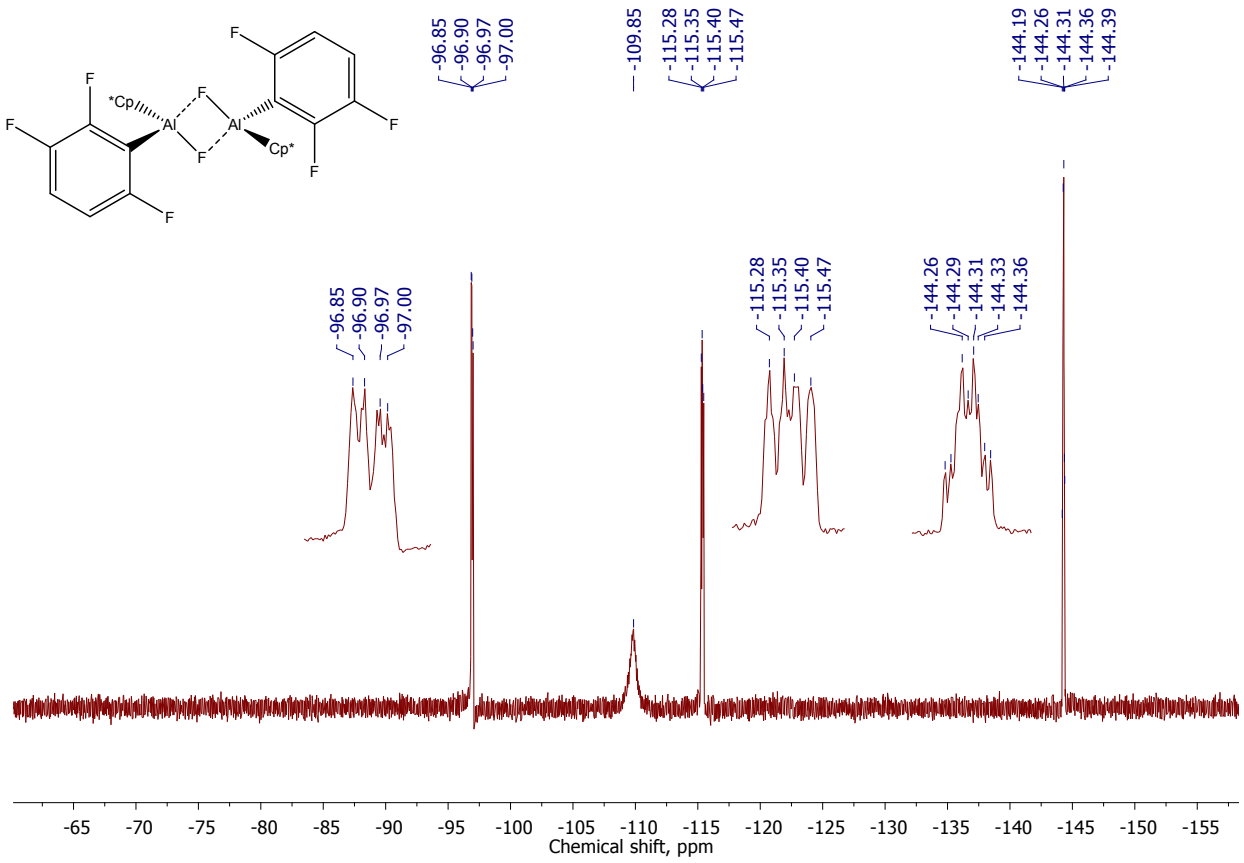

Figure S21. ^{19}F NMR spectrum (377 MHz) of $\{Cp^*(C_6F_3H_2)AlF\}_2$ (**4e**) in C_6D_6 and its magnified sections.

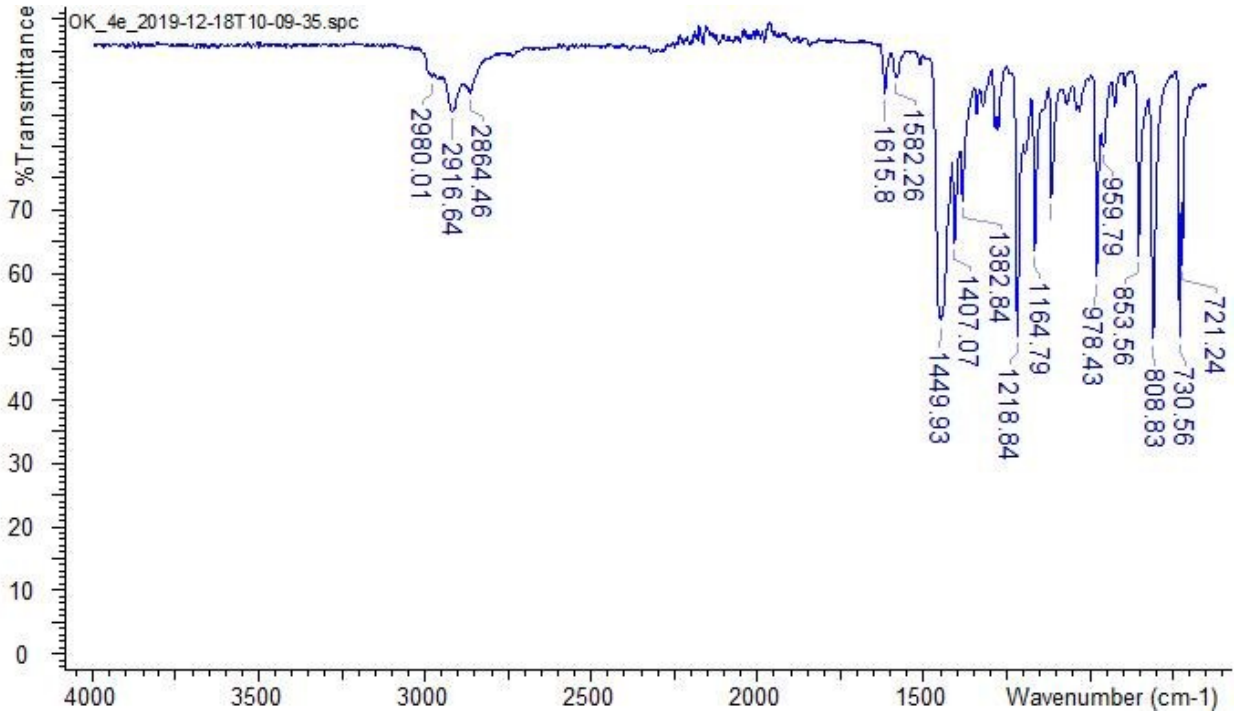

Figure S22. ATR-IR spectrum (diamond) of $\{Cp^*(C_6F_3H_2)AlF\}_2$ (**4e**).

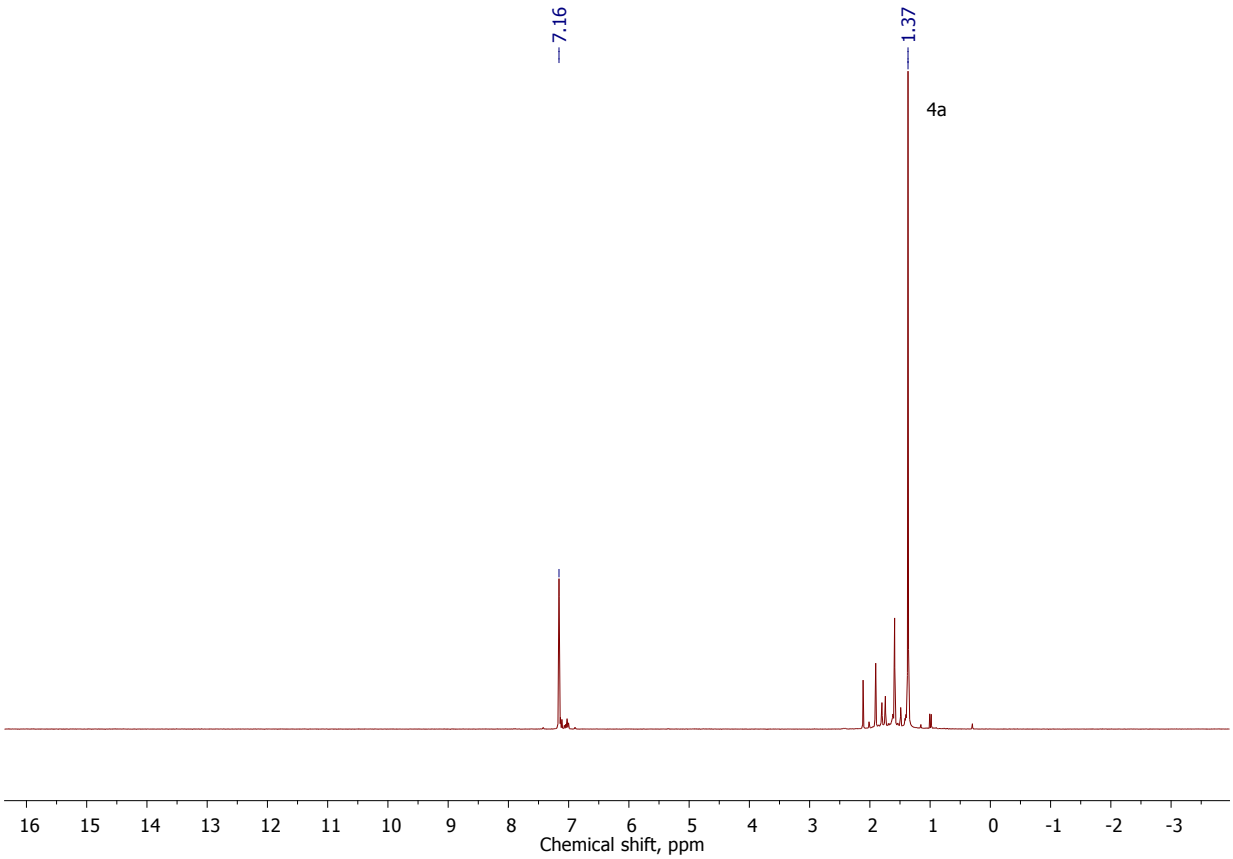

Figure S23. ^{1}H NMR spectrum (300 MHz) of the final reaction mixture from the synthesis of $\{Cp^*(C_5F_4N)AlF\}_2$ (**4a**) in C_6D_6 (peak of solvent at 7.16 ppm).

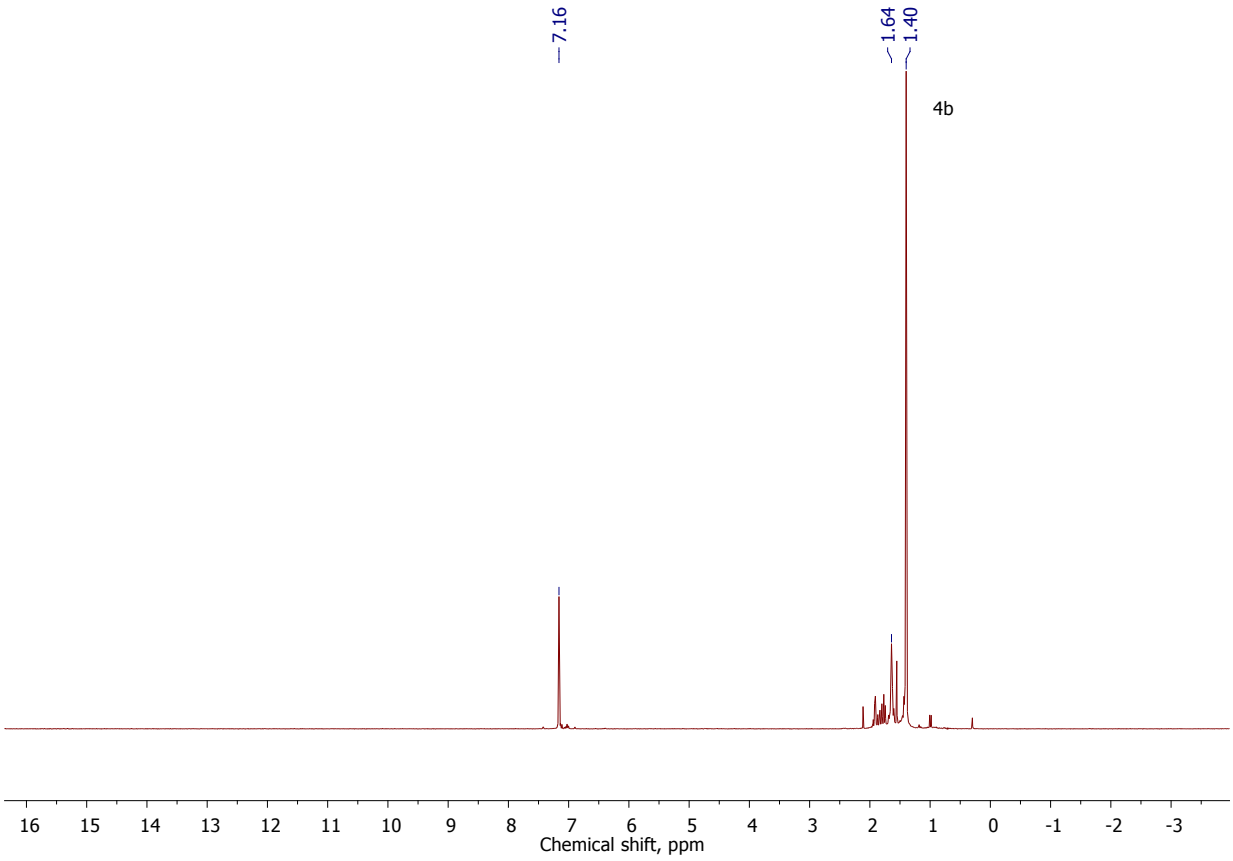

Figure S24. ^{1}H NMR spectrum (300 MHz) of the final reaction mixture from the synthesis of {Cp*(C_7F_7)AlF}$_2$ (**4b**) in C_6D_6 (peak of solvent at 7.16 ppm).

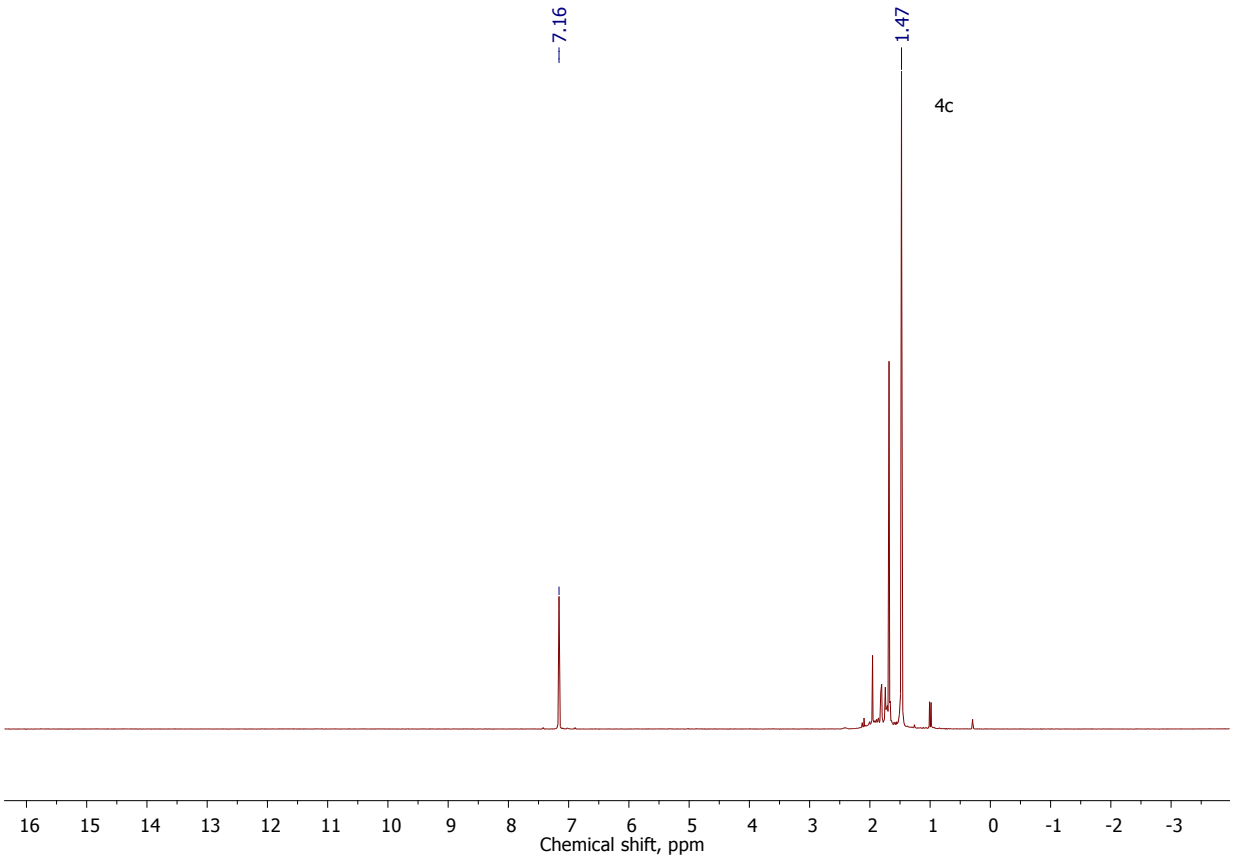

Figure S25. ^{1}H NMR spectrum (300 MHz) of the final reaction mixture from the synthesis of {Cp*(C_6F_5)AlF}$_2$ (**4c**) in C_6D_6 (peak of solvent at 7.16 ppm).

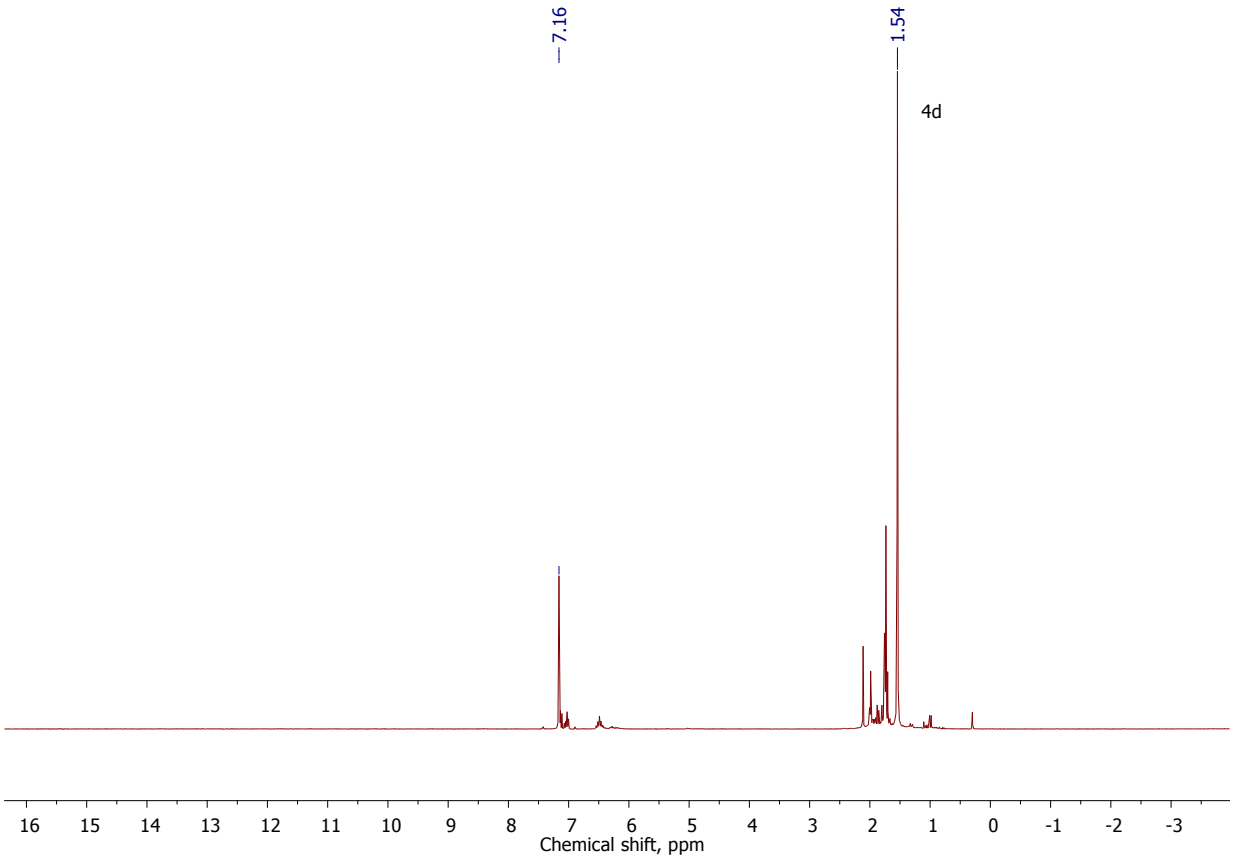

Figure S26. ^{1}H NMR spectrum (300 MHz) of the final reaction mixture from the synthesis of $\{Cp^*(C_6F_4H)AlF\}_2$ (**4d**) in C_6D_6 (peak of solvent at 7.16 ppm).

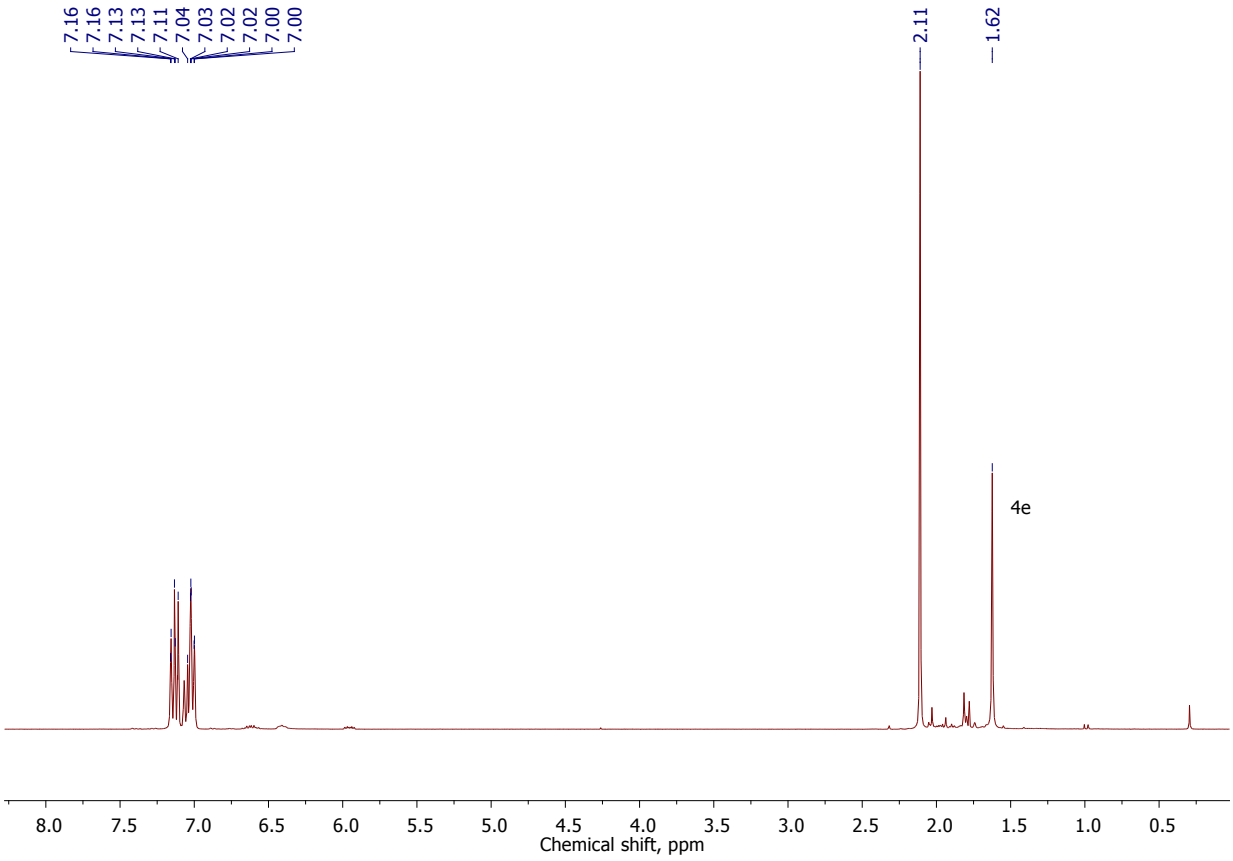

Figure S27. ^{1}H NMR spectrum (300 MHz) of the final reaction mixture from the synthesis of {Cp*($C_6F_3H_2$)AlF}$_2$ (**4e**) in C_6D_6 (peaks at 2.11 ppm and in aromatic region belong to toluene, which was used as a solvent and was not removed completely).

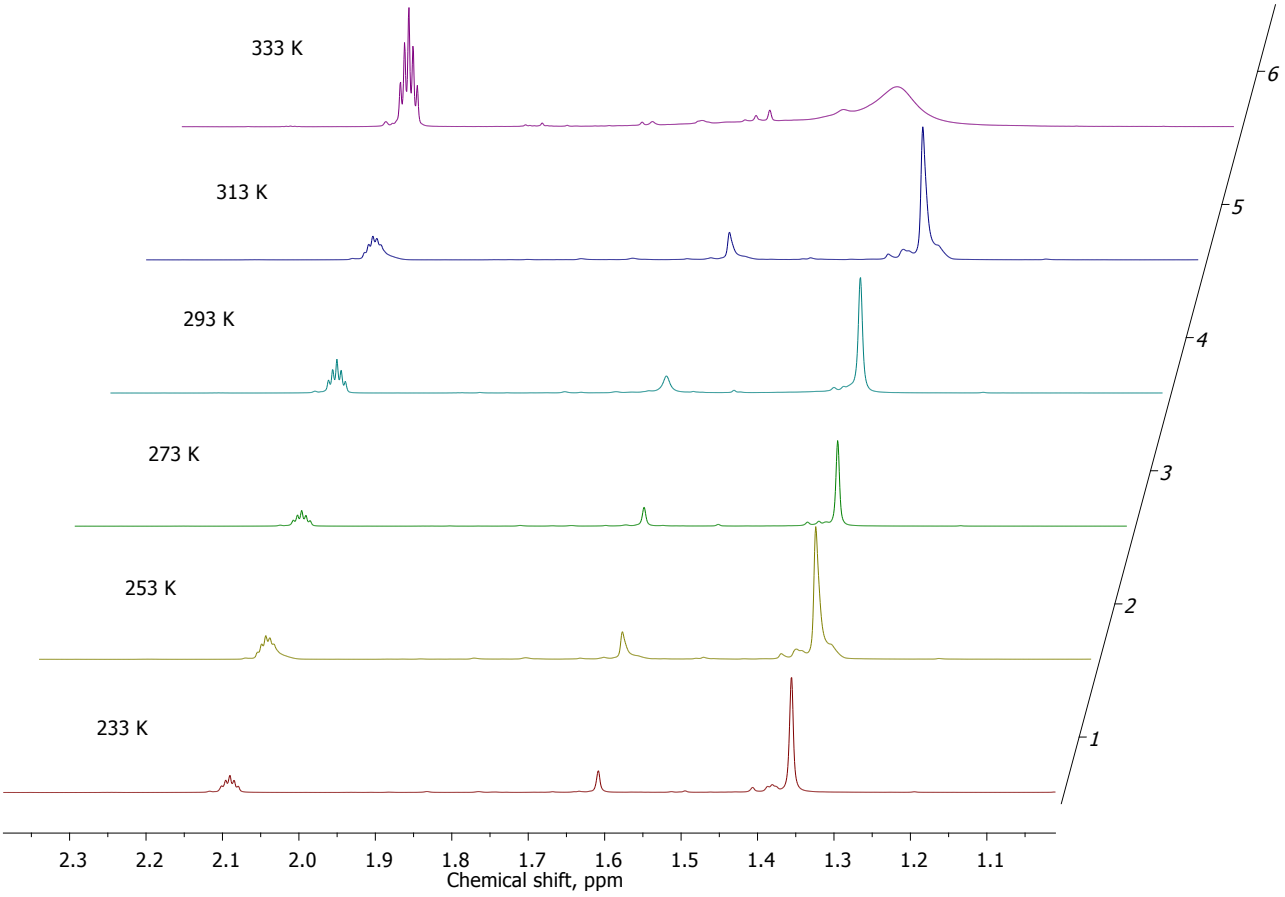

Figure S28. Different temperatures ^{1}H NMR spectra (400 MHz) of $\{Cp^*(C_7F_7)AlF\}_2$ (**4b**) in Tol-d8 (solvent peak at 2.09 ppm).

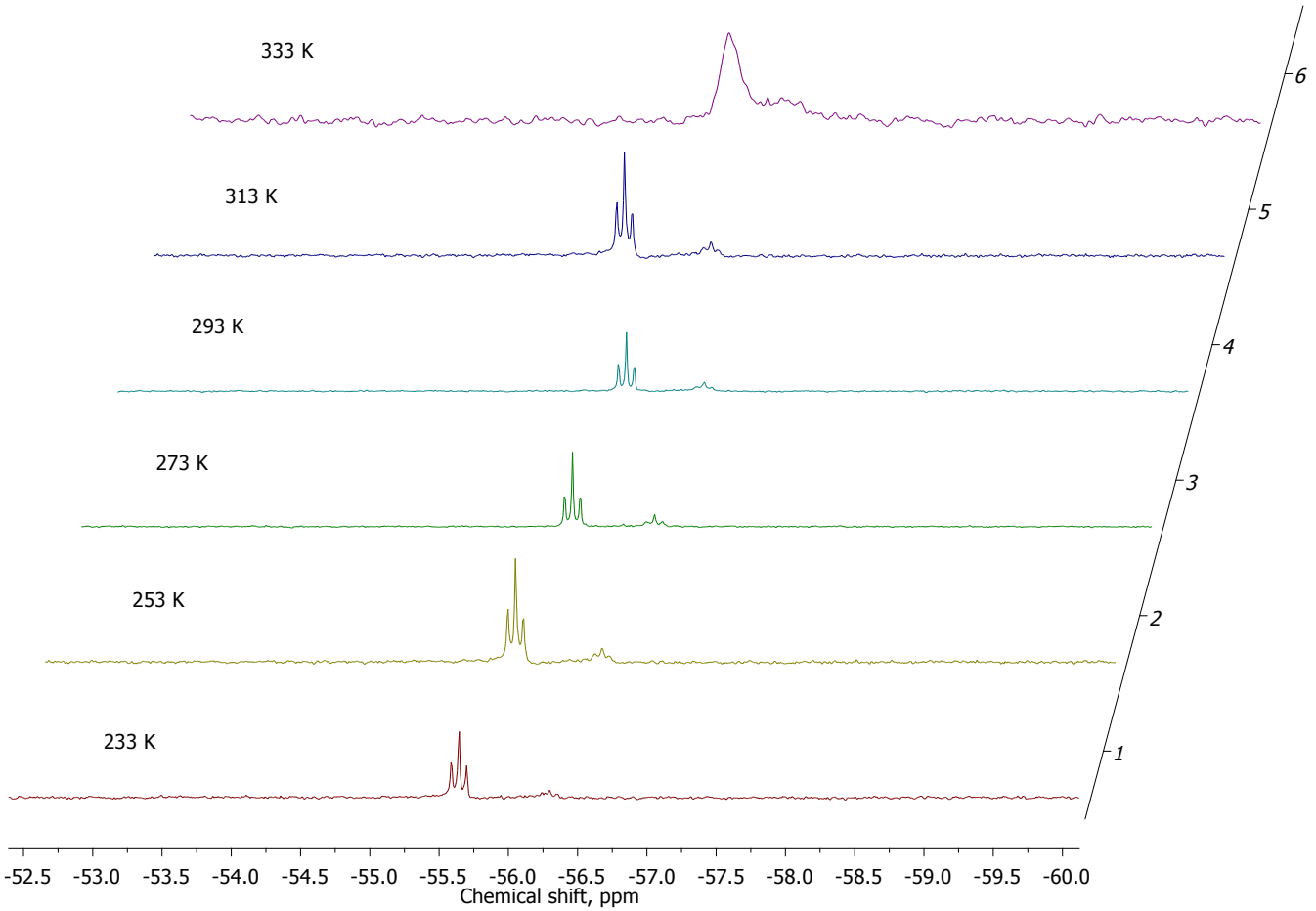

Figure S29. Different temperatures ^{19}F NMR spectra (377 MHz) of $\{Cp^*(C_7F_7)AlF\}_2$ (**4b**) in Tol-d8 in the region of $-CF_3$ group chemical shift.

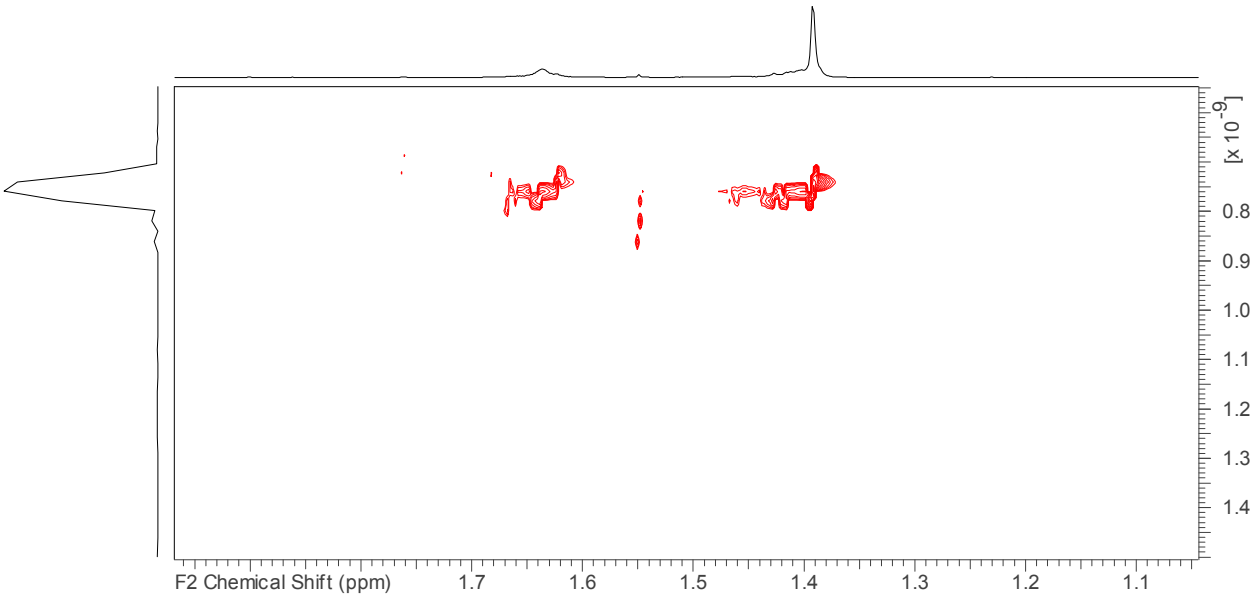

Figure S30. ^{1}H DOSY NMR spectrum (400 MHz) of the {Cp*(C_7F_7)AlF}$_2$ (**4b**) in C_6D_6.

Computational details

Calculations were performed with the Gaussian 16 program package[8] and the M06-2X hybrid functional[9] using 6-31G(d) basis sets[10] for geometry optimizations and frequency calculations. The absence of imaginary frequencies confirmed stationary points as minima, while optimized structures were identified as transition states when having only one imaginary frequency. For single-point calculations, 6-311+G(d,p) basis sets[10b,11] and the SMD solvation model were applied in order to estimate solvent effects.[12] Benzene has been chosen to allow for a comparison with the recent computational investigation about C–F bond activation by **2**.[13] Thermal corrections obtained at the M06-2X/6-31G(d) level of theory were calculated for standard conditions, i.e.298.15 K and 1 bar. All energies are given in kJ mol^{-1}. Please note that in case of **Int1** only certain isomers could be located on the potential-energy surface as minima and are hence given in Table 1.

In order to check that the presented results are not dependent on the computational method a, we have performed additional calculations for the **1'**/**3c** couple using the following protocols, which have been applied before to investigate the activation of C–F bonds by **2**:[14] b) B3YLP/6-31G(d,p),[10,15] c) B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d,p),[10,11,15,16,17] and d) B3PW91-D3/6-311++G(d,p)//B3PW91-D3/6-31G(d,p).[10,11,16,17,18] In the latter two cases, the SMD[12] and PCM[19] solvent models (benzene) have been included in the single-point calculations. The results are given in Table S2.

In brief, only by using methods **a** and **c** we have been able obtain a tetramerization enthalpies close to the experimental value of -150 kJ mol^{-1},[20] while the other methods gave significant lower (**d**) or higher (**b**) values. While, all methods overestimate entropic contributions, formation of the tetramer is endergon with methods **a**-**c**, while it is exergon according to method **d**. Although ΔG_{tetra} gives in the latter case values close to the experiment (-60.6 kJ mol^{-1} at 298K),[20] this is only caused by the significant error in the calculation of ΔH_{tetra}.

With respect to the reaction of **1'** with **3c**, comparable trends and energies are observed for all four methods, justifying the computational protocol. In this respect, decreasing activation energies in the order **b** > **c** > **d** were observed also for the **2**/**3c** couple.[14c]

Table S2. Comparison of the computational protocol for the **1'**/**3c** couple with other approaches.

Method	**a**	**b**	**c**	**d**
Functional-Disp.	M062x	B3LYP	B3LYP-D3	B3PW91-D3
Geom + Freq	6-31G(d,p)	6-31G(d,p)	6-31G(d,p)	6-31G(d,p)
SP	6-311+G(d,p)	6-31G(d,p)	6-311++G(d,p)	6-311++G(d,p)
Solvent model	SMD (benzene)	-	SMD (benzene)	PCM (benzene)
¼ **1** + **3c**	20.5 (-159.8)	116.6 (-37.2)	16.8 (-146.5)	-73.2 (-245.2)
1' + **3c**	0.0	0.0	0.0	0.0
4c_Int1	30.4 (-21.5)	27.3 (-10.9)	28.7 (-18.5)	24.4 (-23.3)
4c_TS	132.8 (80.5)	134.9 (84.7)	122.5 (69.8)	114.8 (61.4)
4c_Int2	-311.9 (-363.6)	-285.0 (-333.7)	-310.1 (-357.9)	-314.1 (-362.2)
4c	-409.0 (-529.8)	-350.0 (-459.1)	-390.2 (-507.9)	-407.5 (-530.3)
4c'	-394.3 (-525.3)	-344.4 (-446.4)	-385.5 (-502.9)	-404.6 (-525.9)

The coordinates of the optimized structures are given in the following:

1

0 1

C	1.326810	-2.428243	-2.741023
C	1.580385	-3.099387	-1.511533
C	2.721173	-2.505616	-0.902612
C	3.166378	-1.455032	-1.749996
Al	1.010148	-0.932936	-0.986175
C	2.305626	-1.404064	-2.883157
C	2.501499	-0.456300	-4.029904
H	2.492111	0.589268	-3.696951
H	3.467713	-0.634298	-4.516929
H	1.723343	-0.568283	-4.788306
C	4.358237	-0.563698	-1.561566
H	4.960348	-0.528947	-2.476495
H	4.069775	0.466378	-1.319116
H	5.000581	-0.923853	-0.753937
C	0.227473	-2.785117	-3.700559
H	0.296824	-2.198410	-4.620157
H	0.283643	-3.842205	-3.981741
H	-0.767651	-2.611289	-3.270684
C	3.308031	-2.932035	0.411859
H	4.364052	-2.655568	0.484913
H	2.786723	-2.472368	1.263840
H	3.240249	-4.017985	0.532878
C	-1.270204	-2.771069	2.425455
C	-2.238847	-2.937628	1.395393
C	-3.125376	-1.824149	1.438533
C	-2.706802	-0.964911	2.490617
Al	-0.983915	-1.010626	0.929975
C	-1.555998	-1.546208	3.092445
C	-2.402006	-4.089064	0.446840
H	-3.366544	-4.585697	0.605944
H	-1.618734	-4.839055	0.577960
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H	-0.640262	0.101160	4.129140
H	-1.351535	-1.120601	5.196286
H	0.175096	-1.448325	4.362878
C	-3.326709	0.336433	2.910694
H	-3.261361	0.464625	3.995921
H	-2.827916	1.199255	2.446275
H	-4.384559	0.380691	2.634869
C	-0.152678	-3.704817	2.794087
H	0.833651	-3.249143	2.637145
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H	-0.189615	-4.622944	2.202135
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H	-4.982612	-0.876324	0.897691
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C	2.643018	2.556412	0.970417
C	3.084372	1.513724	1.829664
Al	0.959053	0.954628	1.012227
C	2.197216	1.449162	2.941516
C	2.379983	0.503757	4.092640
H	2.381059	-0.542564	3.761562
H	3.337491	0.687686	4.594319
H	1.589688	0.612930	4.838831
C	4.294206	0.641483	1.669442
H	4.870974	0.609566	2.600634
H	4.027796	-0.391097	1.412791
H	4.953499	1.016202	0.882272
C	0.076675	2.796280	3.705534
H	0.131056	2.209688	4.626183
H	0.110171	3.853779	3.988834
H	-0.904553	2.608175	3.250565
C	3.255200	2.990365	-0.329978
H	4.321145	2.746743	-0.369052
H	2.774413	2.507719	-1.193036
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H	0.512453	4.128540	-0.093481

1'

0 1

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C	0.896878	-0.814152	-0.272152
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H	-1.261541	-2.810704	-1.340186
H	-0.480103	-3.210910	0.192539
C	2.008431	-1.822701	-0.308529
H	1.720367	-2.754992	0.185158
H	2.283411	-2.066912	-1.341101
H	2.905823	-1.448664	0.192214
C	2.354924	1.345792	-0.307802
H	3.150707	0.785464	0.190766
H	2.675150	1.526698	-1.340309
H	2.275946	2.317175	0.188223
C	-0.552765	2.655384	-0.308369
H	0.226963	3.239922	0.187901
H	-0.629102	3.015429	-1.340810
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3a

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C	1.198569	0.419998	0.000103
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C	-1.126467	-0.968039	-0.000091
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F	2.359856	1.061186	-0.000058
F	-0.000112	2.442810	-0.000011
F	-2.359816	1.061199	-0.000076
F	-2.258170	-1.653332	-0.000013

3b

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C	-0.003470	-1.156947	-0.000048
C	1.379460	-1.235086	0.000019
C	2.125199	-0.061522	0.000008
C	1.485758	1.169260	0.000016
C	0.095561	1.231484	-0.000012

C	-2.176101	0.041787	0.000011
F	-2.632371	-0.604129	-1.078036
F	-2.632265	-0.605252	1.077473
F	-2.703904	1.263923	0.000676
F	-0.458678	2.436599	-0.000067
F	2.201050	2.287384	0.000003
F	3.447762	-0.120722	0.000029
F	1.991934	-2.412064	0.000006
F	-0.706081	-2.284053	-0.000074

3c

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C	1.192034	-0.713617	0.000022
C	-0.021998	-1.389173	-0.000003
C	-1.214140	-0.675524	0.000022
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F	0.042854	2.716385	-0.000001
F	-2.330904	1.395470	-0.000013
F	-2.374122	-1.320882	0.000001
F	-0.043048	-2.716380	-0.000015
F	2.331002	-1.395307	0.000002

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C	-1.205240	0.422925	0.000002
C	-1.191658	-0.966236	0.000007
C	0.000037	-1.674097	0.000003
H	0.000005	-2.756867	0.000003
F	-2.356728	-1.610988	-0.000005
F	-2.353706	1.092363	-0.000004
F	-0.000099	2.441151	0.000000
F	2.353724	1.092350	-0.000004
F	2.356805	-1.610833	-0.000005

3e

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C	-0.696990	-1.729930	0.000002
C	-1.379795	-0.526300	0.000000
C	-0.693500	0.684155	-0.000001
C	0.693501	0.684155	0.000002
C	1.379794	-0.526301	-0.000003
H	1.264136	-2.653053	-0.000006
H	-1.264141	-2.653051	0.000008
F	2.713663	-0.493208	0.000001
F	1.356281	1.836040	0.000001
F	-1.356279	1.836042	-0.000001
F	-2.713664	-0.493206	0.000000

3f

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C	-0.076360	1.363495	0.000001
C	-1.256551	0.634530	-0.000005
C	-1.142641	-0.747877	-0.000008
C	0.078743	-1.405482	-0.000000
C	1.219032	-0.615622	0.000012
C	1.177790	0.770910	0.000005
H	-2.222559	1.122445	0.000009
H	0.139186	-2.486030	0.000006
H	2.083332	1.363567	0.000003
F	-2.260427	-1.479488	0.000003
F	2.411521	-1.217775	-0.000007
F	-0.151099	2.697296	-0.000001

3g

0 1

C	-0.658415	-1.398407	0.000009
C	0.533638	-0.695411	0.000032
C	0.533639	0.695410	0.000007
C	-0.658413	1.398406	-0.000002
C	-1.862548	0.695962	0.000007
C	-1.862548	-0.695961	-0.000016
H	-0.622816	-2.482271	-0.000001
H	-0.622814	2.482270	-0.000017
H	-2.799742	1.241813	0.000003
H	-2.799742	-1.241812	-0.000036
F	1.705166	-1.338050	-0.000013
F	1.705166	1.338050	-0.000006

3h

0 1

C	-0.929486	-0.000015	-0.000020
C	-0.260684	1.214689	-0.000064
C	1.131447	1.205702	-0.000095
C	1.829725	0.000006	0.000175
C	1.131459	-1.205684	-0.000090
C	-0.260684	-1.214707	-0.000065
F	-2.271535	0.000008	0.000100
H	-0.831675	-2.136477	-0.000113
H	1.670983	-2.147491	-0.000054
H	2.914603	0.000003	0.000368
H	1.670963	2.147513	-0.000052
H	-0.831720	2.136432	-0.000100

4a_2-Int1

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C	-2.781933	-0.980246	0.425476
C	-1.826127	-0.270284	1.208731
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C	-3.259601	-0.105132	-0.591567
C	-2.591271	1.143347	-0.443028
C	-4.311987	-0.427649	-1.612772
H	-4.308935	-1.490439	-1.870207
H	-5.311005	-0.181767	-1.235159
H	-4.160520	0.136759	-2.537096
C	-2.809834	2.373454	-1.275496
H	-3.090995	2.121495	-2.301856
H	-3.610591	2.993385	-0.855876
H	-1.906748	2.988860	-1.320850
C	-0.844845	2.159784	1.185166
H	-1.447672	2.899992	1.723593
H	-0.079583	1.797788	1.875834
H	-0.331814	2.685101	0.372894
C	-1.116386	-0.828201	2.409600
H	-0.276854	-0.200325	2.715049
H	-1.801459	-0.903158	3.261841
H	-0.717202	-1.828952	2.216342
C	-3.237421	-2.388768	0.675553
H	-2.436867	-2.993974	1.110372
H	-4.082447	-2.408397	1.373525
H	-3.560147	-2.878612	-0.247351
Al	-1.010922	-0.458362	-0.953574
C	2.152103	0.218720	1.331406
C	2.379136	-1.568818	-0.014707
C	2.615208	-0.782660	-1.135990
C	2.590725	0.594046	-0.968948
C	2.355745	1.120101	0.295980
F	1.932309	0.703518	2.549955
F	2.317271	2.432832	0.491261
F	2.761817	1.396868	-2.002739
F	2.794793	-1.316129	-2.335063
F	2.361885	-2.882667	-0.163999
N	2.160115	-1.084868	1.185498

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C	2.788333	-1.060717	0.199972
C	3.141177	0.286718	-0.120212
C	2.269156	1.155935	0.611744
C	1.733777	-1.019960	1.175447
C	1.429969	0.340103	1.434069
C	1.044871	-2.198409	1.802543
H	1.319802	-3.131207	1.305174
H	1.320011	-2.290026	2.858545
H	-0.044204	-2.106415	1.743291
C	0.353000	0.835353	2.352934
H	-0.434298	0.085142	2.476100
H	0.755682	1.061956	3.346357
H	-0.112539	1.747505	1.967411
C	2.285443	2.659303	0.597603
H	2.923379	3.048393	1.398247
H	2.666414	3.047520	-0.350361

H	1.281992	3.068064	0.740953
C	4.210028	0.687479	-1.093784
H	4.125727	1.742322	-1.364300
H	5.204293	0.531188	-0.661229
H	4.144307	0.104417	-2.016381
C	3.470204	-2.279743	-0.354633
H	3.729874	-2.140285	-1.407959
H	4.395573	-2.490007	0.192613
H	2.833853	-3.165174	-0.285167
Al	1.103082	-0.096258	-0.773965
C	-0.862827	-0.133472	-0.546972
C	-2.797823	-1.348514	-0.298084
C	-3.592145	-0.211919	-0.130691
C	-2.961485	1.017712	-0.167117
C	-1.585619	1.032810	-0.379104
F	1.422800	-0.098709	-2.413666
F	-0.953978	2.220859	-0.397847
F	-3.651403	2.137243	-0.002911
F	-4.902743	-0.302391	0.068174
F	-3.409800	-2.528144	-0.245916
N	-1.507166	-1.328263	-0.493507

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C	3.117739	-0.966179	0.345339
C	2.759648	-0.502062	-0.960958
C	2.330554	0.851974	-0.844299
C	2.926795	0.115642	1.262740
C	2.435673	1.234095	0.530094
C	3.196829	0.065195	2.738492
H	3.036594	-0.939452	3.139549
H	4.232614	0.347227	2.957138
H	2.544047	0.746900	3.289957
C	2.086621	2.586050	1.083705
H	1.967450	2.551623	2.169215
H	2.874862	3.312348	0.858586
H	1.151507	2.960950	0.658606
C	1.849746	1.706410	-1.982297
H	2.669525	1.926125	-2.674383
H	1.056153	1.204464	-2.544210
H	1.448773	2.655271	-1.619708
C	2.822945	-1.273470	-2.246681
H	1.968537	-1.037296	-2.887376
H	3.736461	-1.027618	-2.799300
H	2.819007	-2.352110	-2.071273
C	3.678033	-2.317909	0.682859
H	3.329963	-3.082637	-0.016037
H	4.772606	-2.302008	0.640679
H	3.390200	-2.632831	1.689349
Al	0.944030	-0.443957	0.291938
C	-1.190101	-0.527360	-0.294429
C	-3.239375	-1.381835	0.220695
C	-3.849110	-0.138720	0.295852
C	-3.043832	0.970872	0.022230
C	-1.735449	0.778419	-0.346781
F	-0.226973	-0.764125	-1.450473
F	-0.904081	1.823802	-0.511955
F	-3.553715	2.193965	0.105210
F	-5.136794	0.012925	0.614461
F	-3.987262	-2.454537	0.461784
N	-1.981652	-1.582075	-0.085229

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Al	-0.927139	1.081065	-0.051795
F	0.004513	-0.059013	-1.173451
C	-2.691352	0.172232	-0.061747
C	-3.453284	-0.028297	1.075913
C	-4.736700	-0.565448	1.017429
C	-5.241771	-0.896860	-0.226672
C	-4.422858	-0.664234	-1.333371
C	-1.511422	3.079466	0.857805
C	-2.016190	3.064680	-0.473800
C	-0.925395	2.870096	-1.362903
C	0.276355	2.817698	-0.579682
C	-0.089849	2.939297	0.795440
C	-2.334414	3.260094	2.101135
H	-3.342337	2.854234	1.974333
H	-2.434633	4.322366	2.350408
H	-1.886923	2.755806	2.961356
C	-3.461690	3.163768	-0.861827
H	-4.106986	2.642628	-0.146275
H	-3.638715	2.722859	-1.846438
H	-3.784943	4.209997	-0.896895
C	-0.992252	2.766825	-2.860537
H	-1.893547	2.238960	-3.185352
H	-0.131513	2.217680	-3.251985
H	-0.995270	3.758950	-3.325495
C	1.671272	2.768230	-1.132485
H	2.401768	2.587155	-0.338873
H	1.923336	3.724672	-1.604459
H	1.787770	1.984333	-1.887500
C	0.857680	2.929970	1.960788
H	1.313670	3.916528	2.098539
H	1.658997	2.197556	1.824973
H	0.337842	2.671053	2.886428
Al	0.927131	-1.080995	0.051786
F	-0.004479	0.059117	1.173434
C	2.691380	-0.172235	0.061746
C	3.453336	0.028217	-1.075911
C	4.736778	0.565307	-1.017430
C	5.241844	0.896751	0.226665
C	4.422901	0.664213	1.333361
C	1.511357	-3.079421	-0.857792
C	2.016113	-3.064646	0.473816
C	0.925316	-2.870020	1.362908
C	-0.276427	-2.817561	0.579677
C	0.089787	-2.939210	-0.795438
C	2.334353	-3.260075	-2.101114
H	3.342284	-2.854234	-1.974311
H	2.434554	-4.322351	-2.350379
H	1.886877	-2.755786	-2.961343
C	3.461606	-3.163780	0.861855
H	4.106924	-2.642661	0.146307
H	3.638637	-2.722874	1.846466
H	3.784825	-4.210019	0.896928
C	0.992163	-2.766744	2.860542
H	1.893488	-2.238934	3.185363
H	0.131455	-2.217543	3.251978
H	0.995115	-3.758867	3.325506
C	-1.671351	-2.767987	1.132462
H	-2.401826	-2.586872	0.338837
H	-1.923489	-3.724400	1.604454
H	-1.787808	-1.984061	1.887456
C	-0.857732	-2.929861	-1.960793
H	-1.313755	-3.916405	-2.098541
H	-1.659025	-2.197418	-1.824989
H	-0.337878	-2.670969	-2.886431
F	2.948260	-0.261557	-2.287325
F	5.456378	0.763720	-2.112677
F	6.459328	1.412952	0.356054
F	-2.948188	0.261417	2.287333
F	-5.456269	-0.763950	2.112681
F	-6.459220	-1.413147	-0.356060
F	-4.911655	-0.984799	-2.528753
F	4.911737	0.984698	2.528747
N	-3.221218	-0.157190	-1.270749
N	3.221253	0.157187	1.270744

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Al	1.149403	-1.410582	-0.223576
F	1.359822	-0.173867	1.152687
C	-0.826158	-1.576908	-0.124062
C	-2.912231	-1.226025	-1.020489
C	-3.581511	-1.687821	0.114349
C	-2.806897	-2.119392	1.174125
C	-1.424119	-2.049660	1.031024
C	1.641467	-3.172835	-1.572232
C	1.332154	-3.711159	-0.292589
C	2.224261	-3.145908	0.655146
C	3.135864	-2.290661	-0.052822
C	2.776718	-2.317916	-1.435604
C	0.885514	-3.455006	-2.840200
H	-0.180194	-3.222177	-2.734112
H	0.970652	-4.509654	-3.123526
H	1.269649	-2.852905	-3.667699
C	0.210383	-4.667716	-0.020090

H	-0.651219	-4.455629	-0.661771
H	-0.123638	-4.611907	1.018914
H	0.524997	-5.698462	-0.218174
C	2.300115	-3.421049	2.129590
H	1.378315	-3.874243	2.499026
H	2.463968	-2.498030	2.695649
H	3.128533	-4.102062	2.356511
C	4.307113	-1.606400	0.591942
H	4.982078	-1.183272	-0.155123
H	4.879568	-2.322265	1.191411
H	3.993297	-0.796288	1.259670
C	3.462031	-1.602813	-2.566711
H	3.642160	-2.292245	-3.397089
H	4.432339	-1.210468	-2.251691
H	2.869675	-0.764901	-2.948987
Al	1.146564	1.412417	0.223357
F	1.359964	0.176083	-1.152785
C	-0.829307	1.575214	0.123651
C	-1.428117	2.047408	-1.031218
C	-2.811016	2.115111	-1.174145
C	-3.584901	1.682043	-0.114436
C	-2.914787	1.220974	1.020203
C	2.217784	3.150263	-0.654804
C	1.324781	3.713120	0.293530
C	1.635497	3.174596	1.572753
C	2.772476	2.322060	1.435266
C	3.131280	2.296429	0.052390
C	2.292785	3.426627	-2.129064
H	1.370260	3.878858	-2.497851
H	3.120191	4.108964	-2.355696
H	2.457737	2.504292	-2.695915
C	0.201296	4.667925	0.021988
H	-0.132995	4.612173	-1.016937
H	-0.659729	4.453997	0.663835
H	0.514262	5.699072	0.220578
C	0.879348	3.454533	2.841101
H	-0.185951	3.219796	2.735119
H	1.264775	2.852570	3.668097
H	0.962606	4.509147	3.125114
C	3.459648	1.607694	2.565716
H	4.431657	1.219543	2.250709
H	3.636603	2.296468	3.397310
H	2.870187	0.766956	2.946255
C	4.303261	1.614205	-0.593203
H	4.873088	2.330654	-1.194461
H	4.980323	1.193740	0.153483
H	3.990439	0.802441	-1.259386
F	-0.667260	2.443221	-2.067115
F	-3.373848	2.553501	-2.290007
F	-3.665777	-0.763121	-2.019424
F	-3.368969	-2.558231	2.290191
F	-0.662535	-2.443945	2.066959
F	-3.667496	0.756463	2.019037
F	-4.910860	1.666899	-0.189568
F	-4.907487	-1.674496	0.189601
N	-1.617635	1.173679	1.154289
N	-1.615165	-1.176849	-1.154750

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C	-2.676492	-1.086173	-0.361086
C	-1.671529	-1.048722	0.648277
C	-1.657327	0.261588	1.204971
C	-3.289159	0.197759	-0.423392
C	-2.654598	1.032069	0.540388
C	-4.429220	0.590671	-1.317934
H	-4.414545	0.029564	-2.256413
H	-5.392108	0.396861	-0.831806
H	-4.394274	1.654575	-1.568461
C	-3.001526	2.460023	0.847804
H	-3.389349	2.979408	-0.032926
H	-3.767476	2.517715	1.629863
H	-2.127649	3.014805	1.201397
C	-0.784631	0.766370	2.318744
H	-0.369658	1.754225	2.093497
H	-1.356077	0.856288	3.249616
H	0.054752	0.095046	2.515637
C	-0.823077	-2.219937	1.054585
H	0.007274	-1.919078	1.698064
H	-1.417842	-2.952646	1.611938
H	-0.398264	-2.736504	0.187657
C	-3.049925	-2.293562	-1.171402
H	-2.186023	-2.943533	-1.337659
H	-3.816214	-2.886931	-0.659198
H	-3.448172	-2.014869	-2.150920
Al	-1.076779	0.435506	-1.036915
C	2.273605	-0.547756	0.963658
C	2.322468	-1.427682	-0.109167
C	2.512097	0.236788	-1.612584
C	2.468502	1.224090	-0.634741
C	2.339733	0.811487	0.683737
F	2.146583	-0.977702	2.217239
F	2.268751	1.698126	1.661679
F	2.504088	2.512987	-0.941259
F	2.610636	0.614534	-2.874868
F	2.248853	-2.726677	0.142786
N	2.447145	-1.048571	-1.358820

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C	2.332489	-1.155388	0.501578
C	3.072443	-0.103214	-0.129789
C	2.538104	1.142187	0.324256
C	1.396357	-0.551842	1.401874
C	1.509264	0.855759	1.285641
C	0.413466	-1.288686	2.262214
H	0.095371	-2.224254	1.794310
H	0.851307	-1.533629	3.236018
H	-0.482965	-0.687862	2.443312
C	0.669539	1.863308	2.016173
H	-0.363916	1.518155	2.122992
H	1.062651	2.043281	3.022362
H	0.641539	2.821355	1.491763
C	3.031726	2.498356	-0.095175
H	2.274918	3.269475	0.068705
H	3.923069	2.780993	0.475230
H	3.296494	2.512902	-1.156253
C	4.176319	-0.254257	-1.134048
H	4.070167	0.464761	-1.950418
H	5.151919	-0.093158	-0.662458
H	4.178701	-1.253078	-1.575915
C	2.549914	-2.633498	0.330940
H	3.014905	-2.860779	-0.631429
H	3.203961	-3.022893	1.118181
H	1.605221	-3.181593	0.378674
Al	0.996731	0.048358	-0.747097
C	-0.953885	-0.122116	-0.528156
C	-1.591392	-1.350769	-0.415509
C	-3.641688	-0.528260	-0.102787
C	-3.183096	0.780709	-0.182926
C	-1.820705	0.949327	-0.397048
F	1.294950	0.196518	-2.383208
F	-1.347191	2.198783	-0.464211
F	-4.009112	1.816143	-0.056136
F	-4.936028	-0.725678	0.103202
F	-0.822547	-2.450926	-0.511208
N	-2.870662	-1.586512	-0.211737

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C	3.139377	-0.705329	0.339624
C	2.713024	-0.305713	-0.967317
C	2.115858	0.983438	-0.860388
C	2.809934	0.348326	1.249206
C	2.172208	1.386699	0.509439
C	3.093483	0.351987	2.723386
H	3.089470	-0.661579	3.133609
H	4.076018	0.789526	2.931643
H	2.348695	0.932471	3.274311
C	1.656084	2.688384	1.053404
H	1.529844	2.643426	2.137836
H	2.353291	3.504055	0.833816
H	0.687601	2.945045	0.615579
C	1.540481	1.763621	-2.007667
H	1.074632	2.688319	-1.661012
H	2.325835	2.027027	-2.724008
H	0.777485	1.185821	-2.538008
C	2.866111	-1.072764	-2.248254

H	1.972124	-0.975778	-2.871594
H	3.718951	-0.697215	-2.824528
H	3.030992	-2.137287	-2.064207
C	3.866823	-1.972630	0.684594
H	3.602958	-2.784719	0.002314
H	4.950418	-1.824126	0.622365
H	3.635502	-2.304991	1.699962
Al	0.910647	-0.477546	0.307598
C	-1.245521	-0.557483	-0.257990
C	-2.080089	-1.641900	0.087931
C	-3.921741	-0.384139	0.404395
C	-3.254253	0.776069	0.033504
C	-1.929174	0.664767	-0.348949
F	-0.308563	-0.823003	-1.420557
F	-1.231519	1.773297	-0.637345
F	-3.864209	1.959875	0.025387
F	-5.208061	-0.310956	0.737061
F	-1.491519	-2.836832	0.180079
N	-3.333288	-1.560473	0.443144

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Al	0.854894	1.176557	0.040971
F	-0.068803	0.074970	1.205202
C	2.635816	0.312458	0.141357
C	3.324602	-0.197406	-0.945894
C	4.558331	-0.828907	-0.821714
C	5.095951	-0.899141	0.456482
C	3.338013	0.160091	1.331473
C	1.288143	3.066122	-1.064539
C	1.788674	3.230200	0.259258
C	0.703548	3.075466	1.164557
C	-0.491876	2.878985	0.392752
C	-0.128703	2.876652	-0.985463
C	2.089463	3.117981	-2.334189
H	3.084166	2.680830	-2.202756
H	2.224773	4.150880	-2.673963
H	1.591791	2.565394	-3.136095
C	3.225426	3.447053	0.629732
H	3.897515	2.982012	-0.098000
H	3.453640	3.022461	1.611613
H	3.461347	4.516207	0.664159
C	0.742623	3.173116	2.662950
H	1.748188	2.995664	3.050382
H	0.076701	2.436826	3.123706
H	0.421325	4.166177	2.996924
C	-1.869290	2.797166	0.983583
H	-2.621049	2.580679	0.220432
H	-2.134810	3.750473	1.453963
H	-1.936582	2.019392	1.751867
C	-1.040503	2.722405	-2.169516
H	-0.969555	3.602940	-2.816378
H	-2.084165	2.622915	-1.861482
H	-0.792300	1.842015	-2.768794
Al	-0.833658	-1.122161	0.019552
F	0.087435	-0.020317	-1.136605
C	-2.616097	-0.278214	-0.185940
C	-3.485444	-0.060909	0.870405
C	-4.735659	0.520712	0.712361
C	-5.085298	0.887751	-0.581571
C	-3.151876	0.122259	-1.404089
C	-0.837393	-2.922699	1.310090
C	-1.795003	-3.162821	0.286996
C	-1.126018	-3.104499	-0.969080
C	0.268693	-2.897815	-0.720749
C	0.449728	-2.781904	0.688143
C	-1.071468	-2.893524	2.793704
H	-2.121823	-2.710269	3.030833
H	-0.783526	-3.846071	3.252595
H	-0.481878	-2.104575	3.271051
C	-3.267697	-3.366888	0.481931
H	-3.620413	-2.887746	1.399861
H	-3.840799	-2.950886	-0.352351
H	-3.506377	-4.433788	0.550126
C	-1.751718	-3.272735	-2.324489
H	-2.766344	-2.864340	-2.355051
H	-1.169844	-2.757471	-3.093830
H	-1.811774	-4.331097	-2.602197
C	1.326128	-2.842606	-1.786474
H	2.322736	-2.729661	-1.352324
H	1.323069	-3.770127	-2.368216
H	1.170690	-2.009994	-2.478322
C	1.738060	-2.644159	1.446652
H	1.945732	-3.563049	2.006135
H	2.583209	-2.465139	0.776949
H	1.699727	-1.821044	2.167628
F	-3.116997	-0.402314	2.113388
F	-5.554775	0.726584	1.741098
F	-6.264984	1.461159	-0.773345
F	2.808878	-0.100881	-2.176356
F	5.195039	-1.334449	-1.875914
F	6.274455	-1.485763	0.611713
N	4.507822	-0.411905	1.526574
N	-4.319038	0.697042	-1.630924
F	2.759008	0.636258	2.448719
F	-2.416573	-0.088341	-2.506471

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Al	1.070185	-1.424187	-0.068498
F	1.274045	-0.048398	1.162863
C	-0.900625	-1.577667	0.017608
C	-1.784656	-1.341763	-1.023224
C	-3.162927	-1.395134	-0.855563
C	-3.625930	-1.705154	0.417895
C	-1.547737	-1.876495	1.210667
C	1.565176	-3.320571	-1.201343
C	1.250117	-3.703704	0.132369
C	2.142178	-3.031179	1.008806
C	3.059835	-2.270020	0.206829
C	2.702565	-2.457824	-1.163144
C	0.824791	-3.750553	-2.435618
H	-0.259942	-3.691146	-2.294209
H	1.065492	-4.785331	-2.703160
H	1.077650	-3.114903	-3.288515
C	0.125034	-4.614560	0.521860
H	-0.729662	-4.494585	-0.151576
H	-0.221600	-4.415004	1.538710
H	0.441300	-5.662272	0.472076
C	2.209015	-3.127821	2.506050
H	1.275421	-3.509289	2.923769
H	2.395547	-2.147330	2.956295
H	3.019444	-3.797028	2.817018
C	4.229555	-1.514191	0.768969
H	4.908189	-1.185636	-0.021120
H	4.797877	-2.153144	1.453103
H	3.914627	-0.628784	1.332452
C	3.386023	-1.880055	-2.371219
H	3.559653	-2.660908	-3.117718
H	4.358565	-1.456934	-2.107313
H	2.793828	-1.089664	-2.844633
Al	1.058382	1.430757	0.068482
F	1.273850	0.056719	-1.162855
C	-0.913409	1.570211	-0.017876
C	-1.562276	1.865185	-1.210955
C	-3.639464	1.681835	-0.418185
C	-3.174645	1.374383	0.855238
C	-1.796065	1.329030	1.022914
C	2.118458	3.046044	-1.008482
C	1.221681	3.711748	-0.131633
C	1.539791	3.330450	1.201872
C	2.683419	2.475985	1.163112
C	3.041787	2.291346	-0.206960
C	2.184350	3.143902	-2.505691
H	1.247880	3.518630	-2.923076
H	2.989709	3.819311	-2.816427
H	2.378120	2.165059	-2.956459
C	0.089853	4.614384	-0.520767
H	-0.257181	4.410685	-1.536676
H	-0.762863	4.489802	0.154331
H	0.399092	5.664302	-0.473396
C	0.796793	3.754736	2.436556
H	-0.287539	3.687606	2.295578
H	1.054536	3.120621	3.289133
H	1.030205	4.791112	2.704350
C	3.371318	1.902701	2.370780
H	4.346753	1.486603	2.106384
H	3.539642	2.684504	3.117503
H	2.784898	1.107969	2.844105
C	4.216150	1.543139	-0.769615
H	4.777145	2.184140	-1.457842
H	4.899758	1.223331	0.019814
H	3.907000	0.652956	-1.328772
F	-0.789980	2.115012	-2.283812

F	-1.319740	-1.012277	-2.232825
F	-4.004343	-1.108492	-1.845546
F	-0.774013	-2.121737	2.283547
F	-4.014328	1.082905	1.845262
F	-1.329266	1.002413	2.232562
F	-4.948876	1.710900	-0.615798
F	-4.935162	-1.741319	0.615598
N	-2.842933	-1.949069	1.443422
N	-2.857858	1.930220	-1.443704

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C	-3.289342	-0.197394	-0.423332
C	-2.654942	-1.031939	0.540381
C	-1.657491	-0.261714	1.205025
C	-2.676448	1.086430	-0.360819
C	-1.671503	1.048656	0.648538
C	-3.049342	2.294029	-1.171080
H	-3.450369	2.015417	-2.149477
H	-3.813304	2.889253	-0.657547
H	-2.184573	2.942232	-1.339770
C	-0.822817	2.219674	1.054940
H	-0.398346	2.736531	0.188015
H	-1.417342	2.952226	1.612764
H	0.007729	1.918553	1.698034
C	-0.784730	-0.766770	2.318586
H	0.056227	-0.096898	2.513735
H	-1.355370	-0.854477	3.250171
H	-0.371880	-1.755692	2.094127
C	-3.002144	-2.459869	0.847550
H	-2.128230	-3.015105	1.200341
H	-3.767580	-2.517580	1.630108
H	-3.390716	-2.978825	-0.033097
C	-4.429478	-0.589921	-1.317954
H	-5.392344	-0.395006	-0.832227
H	-4.414068	-0.029450	-2.256802
H	-4.395333	-1.654009	-1.567798
Al	-1.076903	-0.435344	-1.036937
C	2.339668	-0.811361	0.683944
C	2.468200	-1.224427	-0.634411
C	2.511975	-0.237450	-1.612580
C	2.322918	1.427590	-0.109736
C	2.273937	0.548013	0.963353
F	2.268551	-1.697537	1.662234
F	2.147248	0.978294	2.216858
F	2.249652	2.726663	0.141814
F	2.610280	-0.615691	-2.874739
F	2.503504	-2.513416	-0.940585
N	2.447338	1.048028	-1.359295

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C	2.179998	-1.235522	0.508311
C	2.991679	-0.242371	-0.130735
C	2.540843	1.041288	0.309290
C	1.283737	-0.561202	1.399422
C	1.491967	0.834643	1.270159
C	0.255025	-1.226005	2.264996
H	-0.133521	-2.134389	1.796216
H	0.681754	-1.506198	3.234164
H	-0.593575	-0.562116	2.454771
C	0.728926	1.906950	1.992491
H	-0.314778	1.616489	2.147671
H	1.168583	2.101485	2.976448
H	0.725420	2.845614	1.433907
C	3.123083	2.360173	-0.115724
H	2.410164	3.176190	0.025895
H	4.018604	2.595576	0.469241
H	3.407873	2.347630	-1.171464
C	4.085851	-0.483518	-1.127935
H	4.081006	0.276686	-1.912939
H	5.065724	-0.461170	-0.638604
H	3.975524	-1.455496	-1.613931
C	2.295218	-2.726722	0.351893
H	2.900363	-3.155503	1.157557
H	1.312865	-3.206123	0.379715
H	2.766848	-2.993456	-0.596985
Al	0.937125	0.041884	-0.755026
C	-1.027392	0.021370	-0.521155
C	-1.752448	-1.149714	-0.393517
C	-3.121499	-1.117284	-0.154684
C	-3.136953	1.130262	-0.151277
C	-1.767587	1.182654	-0.389856
F	1.223512	0.129770	-2.396099
F	-1.161471	2.380169	-0.479192
F	-3.819661	2.262268	-0.026134
F	-3.788830	-2.258963	-0.033585
F	-1.130122	-2.341321	-0.479937
N	-3.798431	0.001853	-0.037412

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C	2.925050	-0.927343	0.428328
C	2.618396	-0.543201	-0.919738
C	2.203613	0.821268	-0.903014
C	2.704316	0.208868	1.270815
C	2.251643	1.285160	0.448112
C	2.934526	0.260902	2.753565
H	2.754041	-0.709878	3.222795
H	3.967844	0.549065	2.974907
H	2.276839	0.988474	3.235809
C	1.909340	2.679583	0.887393
H	1.724928	2.727430	1.963201
H	2.732658	3.364979	0.659033
H	1.014288	3.045236	0.377330
C	1.762621	1.633910	-2.086163
H	0.831813	2.167432	-1.876413
H	2.527307	2.371434	-2.352198
H	1.589904	0.996180	-2.955683
C	2.715718	-1.410034	-2.142831
H	1.835832	-1.294375	-2.782026
H	3.599696	-1.146928	-2.732959
H	2.795417	-2.466297	-1.875674
C	3.455762	-2.260748	0.870488
H	4.549264	-2.277557	0.808939
H	3.178630	-2.478565	1.904951
H	3.074606	-3.073677	0.247509
Al	0.781435	-0.379410	0.275848
C	-1.308414	-0.262234	-0.384572
C	-2.186580	-1.334250	-0.099317
C	-3.456022	-1.077474	0.366435
C	-3.199396	1.133944	0.194963
C	-1.914227	1.012247	-0.282553
F	-0.498847	-0.434308	-1.605020
F	-1.139887	2.103858	-0.476338
F	-3.694264	2.360983	0.349849
F	-4.218704	-2.116376	0.701312
F	-1.690136	-2.582644	-0.111462
N	-3.990467	0.123169	0.493990

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Al	0.894032	-1.111435	-0.038218
F	0.000162	-0.000334	1.129456
F	2.572036	0.170394	2.356138
F	4.880676	1.530154	2.295457
F	2.978051	-0.375325	-2.321388
F	5.321627	0.932629	-2.165798
N	5.099771	1.230692	0.064653
C	2.640273	-0.154922	0.009680
C	3.194841	0.340878	1.177100
C	4.403559	1.031892	1.159705
C	3.409416	0.058823	-1.121173
C	4.617098	0.742322	-1.055917
C	1.963214	-3.092411	-0.282526
C	1.391928	-3.011053	1.020522
C	-0.028271	-2.903345	0.878311
C	-0.326526	-2.871464	-0.515931
C	0.914448	-2.966256	-1.234442
C	3.426161	-3.218002	-0.586825
H	3.723405	-4.271374	-0.630446
H	4.034847	-2.732460	0.182183
H	3.675639	-2.759562	-1.547921
C	2.136477	-3.067797	2.324117
H	2.333781	-4.104299	2.619483
H	1.562915	-2.594748	3.125895
H	3.099874	-2.552104	2.262719
C	-1.001754	-2.853792	2.021565

H	-0.921861	-3.764843	2.623443
H	-2.032160	-2.781999	1.665382
H	-0.822417	-1.997519	2.677544
C	-1.677862	-2.859241	-1.170344
H	-1.871217	-3.825108	-1.650126
H	-1.748344	-2.086465	-1.943035
H	-2.475237	-2.683024	-0.443891
C	1.032010	-3.002796	-2.731507
H	0.805882	-4.003916	-3.115413
H	2.037999	-2.734193	-3.061127
H	0.333042	-2.302657	-3.199278
Al	-0.893599	1.111101	-0.038112
F	0.000058	-0.000094	-1.215311
F	-2.978260	0.376466	-2.321209
F	-5.321930	-0.931364	-2.165732
F	-2.571424	-0.171292	2.356005
F	-4.880128	-1.530882	2.295167
N	-5.099649	-1.230431	0.064542
C	-2.640115	0.155136	0.009709
C	-3.409458	-0.058140	-1.121104
C	-4.617151	-0.741609	-1.055919
C	-3.194455	-0.341198	1.177007
C	-4.403218	-1.032142	1.159537
C	-1.963385	3.092435	-0.281819
C	-0.914476	2.966590	-1.233577
C	0.326375	2.871382	-0.514903
C	0.027831	2.902753	0.879369
C	-1.392320	3.010633	1.021298
C	-3.426222	3.218355	-0.586415
H	-3.722994	4.271813	-0.631178
H	-3.675804	2.758989	-1.547051
H	-4.035197	2.733919	0.183063
C	-1.031805	3.003898	-2.730640
H	-0.805757	4.005252	-3.113980
H	-0.332667	2.304116	-3.198689
H	-2.037728	2.735342	-3.060540
C	1.677854	2.859984	-1.169038
H	1.871240	3.826418	-1.647660
H	2.475097	2.682926	-0.442639
H	1.748543	2.088122	-1.942630
C	1.001188	2.852687	2.022712
H	0.921163	3.763423	2.625043
H	0.821903	1.996059	2.678243
H	2.031636	2.781203	1.666582
C	-2.137363	3.066377	2.324666
H	-2.336029	4.102614	2.620050
H	-3.100124	2.549559	2.262916
H	-1.563485	2.593981	3.126602

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Al	1.008909	-1.412115	-0.161201
F	1.206097	-0.120355	1.155663
C	-0.969619	-1.573891	-0.065630
C	-1.835192	-1.285700	-1.106356
C	-3.213613	-1.365617	-0.933633
C	-2.979296	-2.029771	1.198992
C	-1.593616	-1.961734	1.108530
C	1.493365	-3.217552	-1.422410
C	1.180563	-3.693512	-0.117452
C	2.078302	-3.088194	0.801867
C	2.997214	-2.276109	0.052991
C	2.636097	-2.365383	-1.325742
C	0.754433	-3.559582	-2.684918
H	-0.330063	-3.538322	-2.534123
H	1.019073	-4.561732	-3.039756
H	0.986234	-2.847815	-3.481760
C	0.056424	-4.628795	0.212838
H	-0.795773	-4.473972	-0.456353
H	-0.294847	-4.488199	1.238120
H	0.377933	-5.670534	0.105711
C	2.146900	-3.290079	2.288562
H	1.207642	-3.683340	2.681839
H	2.351387	-2.346614	2.805146
H	2.946257	-3.993100	2.549310
C	4.167842	-1.560636	0.664273
H	4.841544	-1.171957	-0.102381
H	4.741347	-2.246814	1.296259
H	3.853025	-0.720619	1.293708
C	3.317548	-1.705489	-2.492021
H	3.499798	-2.435388	-3.286488
H	4.285472	-1.291339	-2.198610
H	2.718809	-0.892063	-2.915462
Al	0.989523	1.425048	0.160352
F	1.204599	0.136314	-1.156688
C	-0.990916	1.560220	0.064650
C	-1.620532	1.938930	-1.109533
C	-3.007020	1.988802	-1.199287
C	-3.231547	1.323732	0.934127
C	-1.852087	1.261821	1.106132
C	2.039279	3.113382	-0.801782
C	1.130323	3.708986	0.112893
C	1.444494	3.240084	1.420031
C	2.598509	2.402731	1.329536
C	2.966072	2.315162	-0.047639
C	2.110146	3.312511	-2.288735
H	1.165040	3.686375	-2.687022
H	2.896826	4.030075	-2.548429
H	2.334923	2.371639	-2.801592
C	-0.004711	4.628673	-0.223890
H	-0.350851	4.480454	-1.249823
H	-0.856968	4.464965	0.443097
H	0.303023	5.674791	-0.118979
C	0.696257	3.574159	2.679141
H	-0.387227	3.542064	2.523094
H	0.931314	2.864249	3.476704
H	0.949155	4.578697	3.035763
C	3.283560	1.753742	2.499817
H	4.255847	1.347308	2.210141
H	3.457304	2.488384	3.291837
H	2.691389	0.936497	2.925085
C	4.148225	1.613426	-0.652654
H	4.715092	2.305225	-1.284479
H	4.824074	1.235751	0.117607
H	3.846781	0.767526	-1.280731
F	-0.888483	2.260311	-2.193514
F	-3.573780	2.356889	-2.341587
F	-1.355778	-0.875397	-2.293816
F	-4.010727	-1.037502	-1.943555
F	-3.540559	-2.406307	2.341250
F	-0.856836	-2.274512	2.191818
F	-4.023782	0.986529	1.944881
F	-1.366735	0.859136	2.293798
N	-3.796916	1.685865	-0.194583
N	-3.773618	-1.736176	0.195032

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0 1

C	2.605180	1.541999	0.460135
C	1.911094	0.533799	1.189421
C	2.396456	-0.733194	0.759496
C	3.529320	0.899784	-0.412273
C	3.393885	-0.506740	-0.232541
C	4.499347	1.581238	-1.333857
H	4.113792	2.543190	-1.682708
H	5.452562	1.770499	-0.827443
H	4.710015	0.970682	-2.216332
C	4.192514	-1.575268	-0.921328
H	4.502952	-1.265336	-1.923030
H	5.098976	-1.814736	-0.353298
H	3.614868	-2.498517	-1.024290
C	1.976898	-2.086483	1.259883
H	1.768662	-2.778515	0.436829
H	2.766032	-2.536123	1.873127
H	1.076700	-2.031247	1.876941
C	0.889019	0.810286	2.254207
H	0.372756	-0.099105	2.572968
H	1.366733	1.240229	3.142140
H	0.130147	1.523006	1.915593
C	2.405416	3.020223	0.632007
H	2.988244	3.399546	1.479433
H	2.717023	3.573835	-0.257739
H	1.354075	3.259642	0.819959
Al	1.401344	0.303746	-1.066746
C	-2.011446	-0.203520	1.033594
C	-2.267149	0.343666	-0.222069
C	-2.058451	-0.454176	-1.341458
C	-1.321330	-2.274180	0.047224
C	-1.540408	-1.496578	1.178539
F	-2.199873	0.530778	2.126023
F	-1.267790	-1.983254	2.387037
F	-0.839165	-3.501659	0.174417
C	-1.593758	-1.758686	-1.210169
F	-1.353601	-2.488693	-2.291031

F	-2.239603	0.002722	-2.571294
C	-2.665291	1.795923	-0.279420
F	-2.909162	2.209405	-1.519106
F	-1.685703	2.562864	0.225125
F	-3.760522	2.019581	0.454072

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0 1

C	1.889185	-0.425092	1.425914
C	2.874070	-0.838263	0.466511
C	3.350794	0.331213	-0.200300
C	1.749641	0.982956	1.334645
C	2.622659	1.455983	0.304822
C	0.808462	1.812222	2.156387
H	-0.109968	1.260271	2.382361
H	1.268592	2.092267	3.110465
H	0.525424	2.731714	1.638492
C	2.804494	2.891073	-0.104227
H	1.869919	3.449684	-0.013572
H	3.554160	3.383940	0.523846
H	3.135380	2.971830	-1.142903
C	4.390528	0.348095	-1.281579
H	4.359235	1.282424	-1.846305
H	5.394396	0.247127	-0.854815
H	4.238424	-0.468647	-1.991971
C	3.365710	-2.238087	0.227856
H	3.661992	-2.378500	-0.815492
H	4.236284	-2.458627	0.854892
H	2.594711	-2.978766	0.453993
C	1.110925	-1.313092	2.352784
H	1.465337	-1.204623	3.383311
H	0.042953	-1.067096	2.345735
H	1.205464	-2.365308	2.075191
Al	1.238498	0.034539	-0.664345
C	-0.712415	0.300700	-0.424496
C	-1.601804	-0.762142	-0.233833
C	-2.961640	-0.554634	-0.034647
C	-2.616755	1.810530	-0.212127
C	-1.263519	1.568822	-0.411396
F	1.468753	-0.276794	-2.291111
F	-0.470445	2.642969	-0.596690
F	-3.101954	3.046443	-0.203642
C	-3.475315	0.734302	-0.021178
F	-4.772953	0.942939	0.171376
F	-3.792334	-1.581344	0.146436
C	-1.111474	-2.181765	-0.254411
F	-1.660936	-2.901194	-1.229197
F	-1.340324	-2.819795	0.897477
F	0.238631	-2.218071	-0.451435

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C	2.834199	-1.048684	0.568210
C	2.768145	-0.666390	-0.807849
C	2.971611	0.743137	-0.886385
C	3.098768	0.127334	1.339327
C	3.179598	1.235973	0.442080
C	3.271740	0.185634	2.829682
H	2.659927	-0.565969	3.335472
H	4.316037	0.005965	3.107223
H	2.987433	1.163503	3.227005
C	3.464672	2.661779	0.816843
H	3.115220	2.888663	1.827269
H	4.541056	2.861931	0.784155
H	2.974894	3.360316	0.133331
C	2.976934	1.537671	-2.159982
H	2.787803	2.597639	-1.973246
H	3.945472	1.453386	-2.665022
H	2.205953	1.177431	-2.847104
C	2.535082	-1.569958	-1.984214
H	1.688106	-1.228850	-2.586951
H	3.422195	-1.595658	-2.625712
H	2.321475	-2.590358	-1.659379
C	2.687316	-2.448672	1.094230
H	3.603679	-3.023210	0.922028
H	2.492259	-2.448849	2.169215
H	1.861016	-2.973151	0.607960
Al	1.133744	0.359961	0.263916
C	-0.975237	0.396942	-0.443925
C	-1.844139	-0.709824	-0.236926
C	-3.154093	-0.494074	0.188967
C	-2.846312	1.869009	0.090440
C	-1.559512	1.684525	-0.345792
F	-0.095986	0.286423	-1.632032
F	-0.744316	2.745633	-0.478987
F	-3.322819	3.098612	0.266312
C	-3.683422	0.772706	0.330613
F	-4.952230	0.962596	0.701754
F	-3.932641	-1.541113	0.470406
C	-1.284166	-2.089591	-0.156341
F	-2.066568	-3.014871	-0.711605
F	-1.065124	-2.473017	1.119532
F	-0.076794	-2.162864	-0.764381

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Al	-0.973497	0.996557	0.363759
F	-0.031684	0.391265	-1.087550
C	-2.733503	0.030512	0.284299
C	-3.108080	-0.619108	1.451852
C	-4.342683	-1.225670	1.649248
C	-5.283134	-1.186088	0.630495
C	-4.959211	-0.540933	-0.554334
C	-3.711656	0.052053	-0.723464
C	-1.291028	2.384120	2.113350
C	-2.060737	2.899920	1.032481
C	-1.175983	3.187851	-0.043974
C	0.159160	2.898303	0.393173
C	0.086584	2.399429	1.724783
C	-1.806164	2.000507	3.470614
H	-2.828105	1.613875	3.422589
H	-1.811588	2.870018	4.137759
H	-1.184532	1.228333	3.931008
C	-3.551629	3.065378	1.021314
H	-4.041057	2.301099	1.633950
H	-3.958827	2.985649	0.009486
H	-3.838006	4.044548	1.420842
C	-1.517426	3.840436	-1.353283
H	-2.561928	3.679267	-1.629063
H	-0.898101	3.451663	-2.166817
H	-1.348061	4.921732	-1.292831
C	1.390736	3.179056	-0.417990
H	2.293517	2.847743	0.101398
H	1.485238	4.256259	-0.595622
H	1.360498	2.682223	-1.392779
C	1.232663	1.973022	2.594619
H	1.402119	2.702265	3.394399
H	2.157882	1.890964	2.019302
H	1.048988	1.000970	3.060860
Al	0.973452	-0.996491	-0.363744
F	0.031664	-0.391185	1.087570
C	2.733495	-0.030518	-0.284253
C	3.108098	0.619129	-1.451785
C	4.342734	1.225622	-1.649175
C	5.283198	1.185955	-0.630432
C	4.959244	0.540793	0.554383
C	3.711658	-0.052129	0.723493
C	1.291066	-2.383982	-2.113381
C	2.060738	-2.899832	-1.032502
C	1.175945	-3.187817	0.043892
C	-0.159187	-2.898213	-0.393270
C	-0.086557	-2.399291	-1.724862
C	1.806267	-2.000364	-3.470621
H	2.828204	-1.613726	-3.422538
H	1.811729	-2.869878	-4.137761
H	1.184658	-1.228195	-3.931052
C	3.551631	-3.065289	-1.021246
H	4.041099	-2.301003	-1.633842
H	3.958760	-2.985557	-0.009388
H	3.838037	-4.044453	-1.420764
C	1.517256	-3.840500	1.353187
H	2.561763	-3.679486	1.629033
H	0.897922	-3.451706	2.166704
H	1.347759	-4.921772	1.292664
C	-1.390792	-3.178990	0.417835
H	-2.293549	-2.847611	-0.101558
H	-1.485328	-4.256200	0.595406
H	-1.360567	-2.682214	1.392657

C	-1.232578	-1.972814	-2.594735
H	-1.401936	-2.701961	-3.394625
H	-2.157856	-1.890857	-2.019496
H	-1.048879	-1.000700	-3.060835
F	2.243494	0.706158	-2.482162
F	4.629583	1.840663	-2.790668
F	6.473428	1.752948	-0.790088
F	-2.243503	-0.706010	2.482263
F	-4.629507	-1.840686	2.790761
F	-6.473337	-1.753137	0.790151
F	-5.876755	-0.495253	-1.520899
F	5.876771	0.495041	1.520959
C	-3.486609	0.741152	-2.041781
C	3.486577	-0.741253	2.041783
F	-3.726906	-0.065186	-3.082003
F	-4.284828	1.814055	-2.183075
F	-2.222558	1.176506	-2.163876
F	3.726803	0.065073	3.082028
F	2.222532	-1.176645	2.163800
F	4.284821	-1.814145	2.183063

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Al	1.369676	-1.437702	-0.137332
F	1.614396	-0.137628	1.145460
C	-0.615889	-1.539792	-0.369747
C	-1.075561	-1.393242	-1.668756
C	-2.418574	-1.421734	-2.029349
C	-3.377581	-1.560294	-1.038386
C	-2.962597	-1.715418	0.277887
C	-1.611292	-1.722444	0.603996
C	1.749458	-3.413249	-1.275269
C	1.525725	-3.752108	0.087822
C	2.489811	-3.072588	0.877699
C	3.340083	-2.331090	-0.007119
C	2.869897	-2.537017	-1.344085
C	0.944860	-3.932580	-2.429869
H	-0.127821	-3.924217	-2.205916
H	1.222929	-4.968459	-2.655133
H	1.102043	-3.337440	-3.331919
C	0.424304	-4.647866	0.568498
H	-0.547203	-4.347691	0.158677
H	0.338339	-4.637904	1.656850
H	0.606302	-5.681214	0.253231
C	2.698396	-3.145156	2.363256
H	1.883717	-3.676700	2.857957
H	2.759644	-2.146046	2.807832
H	3.632865	-3.669778	2.593079
C	4.587474	-1.634391	0.449440
H	5.125355	-1.179275	-0.383723
H	5.262864	-2.354180	0.926016
H	4.371184	-0.853238	1.186215
C	3.444786	-1.953778	-2.603444
H	3.984566	-2.716068	-3.175278
H	4.145445	-1.144355	-2.382820
H	2.660446	-1.542727	-3.246302
Al	1.385387	1.424720	0.137279
F	1.615566	0.122055	-1.145430
C	-0.599035	1.546764	0.370080
C	-1.592966	1.737231	-0.603667
C	-2.944220	1.741632	-0.277308
C	-3.360239	1.590575	1.039121
C	-2.402313	1.444811	2.030076
C	-1.059637	1.404966	1.669271
C	2.521907	3.047774	-0.878355
C	1.563817	3.737758	-0.090330
C	1.782898	3.398624	1.273420
C	2.894433	2.511419	1.344579
C	3.364010	2.299082	0.008285
C	2.732423	3.116180	-2.363849
H	1.923077	3.654461	-2.860026
H	3.671890	3.631795	-2.593682
H	2.784824	2.115884	-2.806886
C	0.471384	4.643282	-0.573169
H	0.387300	4.633896	-1.661670
H	-0.503524	4.351925	-0.165078
H	0.662111	5.674993	-0.257712
C	0.982255	3.927509	2.426409
H	-0.090291	3.928735	2.201646
H	1.133280	3.332693	3.329719
H	1.269784	4.961192	2.649881
C	3.462478	1.924406	2.605304
H	4.155396	1.107850	2.386522
H	4.009176	2.682218	3.176521
H	2.673550	1.522018	3.248037
C	4.606167	1.591375	-0.445683
H	5.289728	2.305662	-0.918909
H	5.137247	1.129731	0.388241
H	4.384908	0.813595	-1.184521
F	-3.873232	1.882907	-1.224399
F	-0.196184	-1.198508	-2.671167
F	-2.791087	-1.280687	-3.293945
F	-3.892469	-1.849721	1.225140
F	-2.775856	1.307548	3.294789
F	-0.181700	1.203785	2.671693
C	-1.259053	2.016371	-2.044390
C	-1.279633	-2.005038	2.044518
F	-4.652531	1.596844	1.344466
F	-4.669897	-1.556073	-1.343626
F	-1.826627	-1.124268	2.889888
F	0.048928	-1.983009	2.257108
F	-1.714652	-3.218454	2.415548
F	-1.814651	1.140707	-2.889460
F	-1.682808	3.233785	-2.415479
F	0.069156	1.981778	-2.257423

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C	2.605886	-1.541410	-0.460289
C	1.911724	-0.533399	-1.189725
C	2.396654	0.733737	-0.759610
C	3.529575	-0.898985	0.412454
C	3.393855	0.507530	0.232680
C	4.499428	-1.580315	1.334309
H	4.113522	-2.541911	1.683756
H	5.452512	-1.770247	0.827900
H	4.710437	-0.969345	2.216410
C	4.191416	1.576382	0.922247
H	4.501869	1.266164	1.923850
H	5.097771	1.817093	0.354585
H	3.612766	2.498965	1.025574
C	1.976431	2.086851	-1.259892
H	1.769718	2.779207	-0.436725
H	2.764444	2.536179	-1.874804
H	1.075064	2.031340	-1.875211
C	0.889901	-0.809930	-2.254744
H	0.372853	0.099288	-2.572760
H	1.367927	-1.238771	-3.143035
H	0.131600	-1.523496	-1.916621
C	2.406756	-3.019692	-0.632348
H	2.989906	-3.398656	-1.479711
H	2.718438	-3.573268	0.257393
H	1.355550	-3.259533	-0.820524
Al	1.401244	-0.303034	1.066206
C	-1.541400	1.496248	-1.178657
C	-2.011538	0.202884	-1.033523
C	-2.266867	-0.344344	0.222191
C	-1.594581	1.758451	1.210061
C	-1.322674	2.274046	-0.047411
F	-1.269145	1.983073	-2.387156
F	-0.841249	3.501801	-0.174755
F	-1.354698	2.488704	2.290818
F	-2.199494	-0.531659	-2.125884
C	-2.058529	0.453698	1.341513
F	-2.239200	-0.003214	2.571414
C	-2.664305	-1.796796	0.279629
F	-2.907750	-2.210344	1.519388
F	-1.684513	-2.563326	-0.225118
F	-3.759612	-2.020959	-0.453602

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C	2.619937	-1.532876	0.501368
C	3.631946	-0.736048	-0.125995
C	3.474194	0.610453	0.328586
C	1.892858	-0.687326	1.400791
C	2.405645	0.628349	1.288801
C	0.737882	-1.108933	2.259535
H	0.189028	-1.941337	1.810988
H	1.081394	-1.429559	3.249035
H	0.031067	-0.285937	2.404199
C	1.889406	1.831629	2.022663
H	0.799499	1.799290	2.122556
H	2.311642	1.883276	3.031845

H	2.143184	2.759548	1.505176
C	4.333707	1.772835	-0.082902
H	3.809749	2.723637	0.043490
H	5.247253	1.813722	0.519917
H	4.630049	1.694801	-1.132602
C	4.646913	-1.199938	-1.128179
H	4.787407	-0.461094	-1.921057
H	5.615656	-1.371169	-0.646165
H	4.339017	-2.133791	-1.603676
C	2.406204	-3.010876	0.325372
H	2.924346	-3.574405	1.108371
H	1.344588	-3.267401	0.375023
H	2.784178	-3.356893	-0.639762
Al	1.689372	0.001550	-0.749486
C	-0.218639	0.453972	-0.529988
C	-1.185819	-0.532963	-0.411065
C	-2.536856	-0.282872	-0.186059
C	-1.999994	2.085843	-0.191786
C	-0.667347	1.755225	-0.412285
F	2.007841	0.009511	-2.388429
F	0.213484	2.764295	-0.499607
F	-2.391938	3.352824	-0.083206
F	-0.760677	-1.808714	-0.508624
C	-2.919366	1.055174	-0.085268
F	-4.196716	1.358534	0.125296
C	-3.613135	-1.325977	-0.044660
F	-4.544354	-1.181874	-0.995342
F	-4.233533	-1.207081	1.137232
F	-3.136896	-2.568257	-0.127051

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0 1

C	3.606666	-1.306696	0.287904
C	3.427537	-0.601129	-0.944958
C	3.189185	0.769586	-0.637139
C	3.485663	-0.362066	1.354987
C	3.221017	0.917492	0.784004
C	3.620816	-0.672336	2.817543
H	3.310873	-1.697275	3.038867
H	4.660178	-0.562596	3.145969
H	3.008031	-0.004362	3.428634
C	3.024399	2.207655	1.527917
H	2.787364	2.027555	2.579253
H	3.933311	2.817725	1.492108
H	2.207377	2.793041	1.097655
C	2.956109	1.852293	-1.651578
H	2.706153	2.798516	-1.167569
H	3.854259	2.007894	-2.258585
H	2.132066	1.595884	-2.324160
C	3.490980	-1.167112	-2.333557
H	2.726316	-0.718053	-2.974364
H	4.467996	-0.968580	-2.787934
H	3.335679	-2.248850	-2.336223
C	3.933893	-2.764649	0.434049
H	5.018759	-2.915431	0.455012
H	3.523876	-3.178004	1.359241
H	3.532984	-3.350813	-0.396774
Al	1.534843	-0.461585	0.193469
C	-0.507934	0.140785	-0.476657
C	-1.589075	-0.758513	-0.369765
C	-2.860807	-0.350949	-0.005702
C	-2.082630	1.936138	0.010266
C	-0.822973	1.502835	-0.362569
F	0.430866	-0.160523	-1.624679
F	0.182348	2.393826	-0.418983
F	-2.312248	3.234911	0.196903
F	-1.277955	-2.055020	-0.481757
C	-3.106664	1.014456	0.159092
F	-4.333717	1.441177	0.466228
C	-4.025274	-1.285326	0.195942
F	-5.015630	-0.999646	-0.659059
F	-4.523009	-1.159185	1.433068
F	-3.697727	-2.565630	0.021067

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0 1

Al	0.700929	-1.208772	-0.126196
F	0.244137	0.244543	-1.180463
C	2.509162	-0.625438	0.447933
C	2.898208	-0.482962	1.770062
C	4.159501	-0.044788	2.155534
C	5.101768	0.250462	1.176382
C	4.787863	0.103418	-0.172674
C	3.497950	-0.331198	-0.471177
C	0.643816	-3.335030	0.540429
C	1.486394	-3.280231	-0.607767
C	0.722306	-2.771034	-1.692858
C	-0.622534	-2.569032	-1.231005
C	-0.670325	-2.921926	0.149429
C	1.043213	-3.780435	1.918461
H	2.060225	-3.461693	2.167648
H	1.007164	-4.871953	2.006891
H	0.374324	-3.361441	2.675400
C	2.945858	-3.624877	-0.635972
H	3.417305	-3.430490	0.332324
H	3.483416	-3.041148	-1.389380
H	3.090120	-4.685392	-0.869275
C	1.177576	-2.542664	-3.105902
H	2.266335	-2.491864	-3.172827
H	0.777586	-1.604711	-3.504004
H	0.836077	-3.353168	-3.759620
C	-1.759478	-2.148042	-2.116099
H	-2.678463	-1.998181	-1.543772
H	-1.955907	-2.918918	-2.869621
H	-1.537414	-1.215795	-2.646392
C	-1.869497	-2.891118	1.053359
H	-2.071154	-3.891513	1.450188
H	-2.763018	-2.564501	0.517363
H	-1.732908	-2.213569	1.901033
Al	-0.709612	1.264505	0.027684
F	-0.256850	-0.188110	1.071402
C	-2.553318	0.672815	-0.419059
C	-3.108952	0.821512	-1.680008
C	-4.399237	0.434905	-2.007742
C	-5.198475	-0.138307	-1.023192
C	-4.713841	-0.308058	0.270869
C	-3.407431	0.122480	0.518138
C	-0.187554	3.277374	-0.731033
C	-1.376777	3.431899	0.032992
C	-1.106464	3.006811	1.365501
C	0.277797	2.651072	1.446452
C	0.848677	2.815646	0.150294
C	0.013081	3.605841	-2.183030
H	-0.932220	3.599296	-2.730458
H	0.463906	4.597781	-2.299800
H	0.678412	2.881370	-2.662649
C	-2.708123	3.890314	-0.482662
H	-2.822139	3.669934	-1.548039
H	-3.529782	3.400405	0.048989
H	-2.824056	4.971575	-0.350939
C	-2.084596	2.968170	2.505167
H	-3.088458	2.690785	2.168320
H	-1.781111	2.237393	3.259897
H	-2.157836	3.945710	2.994761
C	0.974150	2.204272	2.700704
H	2.038439	2.030222	2.523665
H	0.889207	2.974439	3.474209
H	0.551456	1.277466	3.098751
C	2.287799	2.662516	-0.249835
H	2.723736	3.644323	-0.466330
H	2.878635	2.203805	0.547209
H	2.401156	2.047990	-1.148937
F	-2.365020	1.355213	-2.664597
F	-4.879439	0.596143	-3.239347
F	-6.427503	-0.503222	-1.368766
F	2.032761	-0.769263	2.753945
F	4.473098	0.097951	3.442169
F	6.296557	0.666810	1.579501
F	3.189844	-0.441726	-1.781591
F	-2.963475	-0.019836	1.782335
C	5.719120	0.435997	-1.304501
C	-5.504580	-0.906468	1.401683
F	5.215539	1.430624	-2.050137
F	6.924535	0.817373	-0.881553
F	5.886028	-0.618682	-2.112945
F	-4.875687	-1.979084	1.906534
F	-6.722563	-1.295840	1.024343
F	-5.648461	-0.028010	2.401704

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Al	-1.633712	1.276518	-0.644752
F	-1.840064	0.520238	1.040453
C	0.341743	1.441013	-0.637539
C	1.207491	0.793408	-1.505367
C	2.589040	0.859826	-1.393306
C	3.153208	1.600382	-0.360045
C	2.344143	2.284824	0.541548
C	0.966315	2.168785	0.358228
C	-2.117961	2.570190	-2.434682
C	-1.800311	3.449885	-1.361758
C	-2.696450	3.185497	-0.292494
C	-3.617553	2.172557	-0.726954
C	-3.259276	1.797989	-2.058123
C	-1.375909	2.468751	-3.736817
H	-0.291507	2.461125	-3.581558
H	-1.608791	3.313946	-4.393751
H	-1.635460	1.548488	-4.267022
C	-0.667405	4.432208	-1.359608
H	0.174545	4.061863	-1.952917
H	-0.301179	4.625538	-0.347806
H	-0.983406	5.387978	-1.791810
C	-2.761201	3.868214	1.043573
H	-1.832239	4.395910	1.267832
H	-2.933477	3.145817	1.848168
H	-3.579785	4.596645	1.068482
C	-4.788657	1.705910	0.089312
H	-5.474110	1.100119	-0.507315
H	-5.348726	2.566076	0.470958
H	-4.475800	1.108798	0.953290
C	-3.946200	0.789334	-2.936599
H	-4.117942	1.208493	-3.932545
H	-4.919995	0.510234	-2.526089
H	-3.357964	-0.126849	-3.055675
Al	-1.633797	-1.276540	0.644571
F	-1.840305	-0.520218	-1.040655
C	0.341681	-1.441008	0.637255
C	0.966498	-2.168656	-0.358459
C	2.344345	-2.284498	-0.541592
C	3.153197	-1.599842	0.360048
C	2.588800	-0.859370	1.393228
C	1.207216	-0.793242	1.505174
C	-2.696065	-3.185875	0.292562
C	-1.799727	-3.450274	1.361644
C	-2.117196	-2.570685	2.434669
C	-3.258554	-1.798425	2.058358
C	-3.617130	-2.172992	0.727231
C	-2.760992	-3.868664	-1.043457
H	-1.831299	-4.394648	-1.268730
H	-3.578277	-4.598580	-1.067560
H	-2.935418	-3.146516	-1.847807
C	-0.666799	-4.432566	1.359118
H	-0.300100	-4.624963	0.347305
H	0.174852	-4.062757	1.953179
H	-0.982984	-5.388758	1.790255
C	-1.374879	-2.469274	3.736654
H	-0.290514	-2.461150	3.581166
H	-1.634712	-1.549277	4.267176
H	-1.607250	-3.314759	4.393394
C	-3.945368	-0.789830	2.937000
H	-4.919180	-0.510648	2.526589
H	-4.117060	-1.209097	3.932910
H	-3.357100	0.126322	3.056144
C	-4.788357	-1.706171	-0.088780
H	-5.348210	-2.566248	-0.470931
H	-5.473956	-1.100916	0.508229
H	-4.475677	-1.108445	-0.952393
F	0.713347	0.014386	-2.478099
F	3.378132	0.139864	-2.191957
F	3.377689	-0.139209	2.191903
F	0.712853	-0.014283	2.477847
F	4.475303	-1.578410	0.247507
F	4.475310	1.579334	-0.247444
C	2.855025	3.034429	1.740098
C	2.855572	-3.034201	-1.739918
F	0.183099	2.804231	1.255894
F	0.183500	-2.804171	-1.256263
F	2.426969	-2.464214	-2.871587
F	2.404930	-4.298327	-1.737348
F	4.186922	-3.081920	-1.784146
F	4.186365	3.081630	1.785073
F	2.425582	2.464651	2.871561
F	2.404884	4.298728	1.737256

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0 1

C	3.529274	0.899582	0.412050
C	3.393903	-0.506955	0.232371
C	2.396390	-0.733458	-0.759590
C	2.605044	1.541735	-0.460292
C	1.910952	0.533509	-1.189523
C	2.405586	3.019992	-0.632172
H	2.716000	3.573409	0.258123
H	2.989631	3.399438	-1.478704
H	1.354520	3.259491	-0.821526
C	0.888862	0.809885	-2.254324
H	0.130065	1.522728	-1.915814
H	1.366585	1.239605	-3.142358
H	0.372483	-0.099519	-2.572885
C	1.976615	-2.086751	-1.259823
H	1.076335	-2.031360	-1.876741
H	2.765578	-2.536542	-1.873168
H	1.768360	-2.778715	-0.436717
C	4.192391	-1.575458	0.921388
H	3.615101	-2.499057	1.023150
H	5.099603	-1.814118	0.354223
H	4.501544	-1.266013	1.923640
C	4.499089	1.581383	1.333607
H	5.451038	1.774123	0.826125
H	4.111744	2.541622	1.685224
H	4.712625	0.969348	2.214352
Al	1.401494	0.303271	1.066760
C	-1.321755	-2.274161	-0.047032
C	-1.593934	-1.758485	1.210325
C	-2.058317	-0.453848	1.341533
C	-2.011500	-0.203442	-1.033543
C	-1.540781	-1.496614	-1.178405
F	-0.839857	-3.501759	-0.174176
F	-1.268355	-1.983480	-2.386870
F	-2.199880	0.530802	-2.126020
F	-2.239229	0.003194	2.571350
F	-1.353839	-2.488423	2.291251
C	-2.266940	0.343933	0.222101
C	-2.664743	1.796286	0.279367
F	-3.760025	2.020120	-0.453994
F	-1.685069	2.562969	-0.225377
F	-2.908350	2.209936	1.519055

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0 1

C	3.067242	-1.257346	0.521481
C	3.895924	-0.257626	-0.084629
C	3.438967	1.021030	0.363588
C	2.153357	-0.592929	1.401884
C	2.369151	0.803622	1.298175
C	1.101318	-1.261715	2.235599
H	0.733933	-2.174341	1.758372
H	1.497097	-1.534902	3.219812
H	0.242822	-0.601982	2.393907
C	1.590353	1.864416	2.020387
H	0.531940	1.596232	2.100169
H	1.973800	2.003819	3.036669
H	1.645517	2.826110	1.505604
C	4.033296	2.344017	-0.030792
H	3.311389	3.156851	0.081277
H	4.901648	2.581464	0.593046
H	4.363529	2.335535	-1.073181
C	5.010565	-0.487041	-1.061802
H	5.009137	0.270195	-1.849758
H	5.981441	-0.450241	-0.555735
H	4.921517	-1.461984	-1.546133
C	3.181649	-2.746329	0.345020
H	3.776646	-3.188298	1.151103
H	2.198037	-3.223721	0.354660
H	3.663070	-3.000628	-0.602355
Al	1.855611	0.042384	-0.751618
C	-0.112714	0.039477	-0.568002
C	-0.846617	-1.130021	-0.464022
C	-2.216618	-1.132971	-0.261751
C	-2.203917	1.257939	-0.253801
C	-0.827161	1.216397	-0.455658
F	2.188521	0.144105	-2.383659
F	-0.172385	2.391096	-0.529092

F	-2.797665	2.444159	-0.154828
F	-2.874751	-2.287193	-0.162694
F	-0.214059	-2.317468	-0.542415
C	-2.918913	0.067596	-0.157538
C	-4.407214	-0.013248	0.064018
F	-4.980694	1.187990	0.123431
F	-4.679057	-0.652459	1.208914
F	-4.995074	-0.698752	-0.922919

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0 1

C	3.839955	-0.864678	0.622928
C	3.651253	-0.508970	-0.754088
C	3.201308	0.843562	-0.799501
C	3.511817	0.276149	1.421121
C	3.109728	1.327466	0.542382
C	3.595157	0.353760	2.918094
H	3.398513	-0.616437	3.382099
H	4.592844	0.676464	3.234817
H	2.872059	1.066123	3.323358
C	2.696229	2.718798	0.926677
H	2.407539	2.774913	1.978948
H	3.522894	3.420108	0.769815
H	1.847162	3.058972	0.328087
C	2.857530	1.626400	-2.033621
H	1.919468	2.173287	-1.908134
H	3.647071	2.349979	-2.263035
H	2.742198	0.966226	-2.896020
C	3.890237	-1.389313	-1.947595
H	3.079643	-1.299717	-2.676417
H	4.825352	-1.116520	-2.447797
H	3.961335	-2.440396	-1.658282
C	4.358123	-2.177801	1.134987
H	5.452565	-2.167760	1.179156
H	3.987575	-2.388874	2.141255
H	4.058614	-3.008621	0.491282
Al	1.699815	-0.379961	0.254672
C	-0.340243	-0.320794	-0.565854
C	-1.199506	-1.425154	-0.362854
C	-2.516707	-1.249616	-0.017080
C	-2.290953	1.110502	-0.209163
C	-0.968458	0.942767	-0.560473
F	0.617010	-0.492914	-1.689961
F	-0.177771	2.032006	-0.687931
F	-2.750717	2.359083	-0.131727
F	-3.254194	-2.326929	0.258714
F	-0.645707	-2.646545	-0.304985
C	-3.120277	0.013261	0.032193
C	-4.578706	0.094753	0.354595
F	-5.044155	1.345247	0.293876
F	-4.836500	-0.370270	1.587876
F	-5.307004	-0.647990	-0.493232

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0 1

Al	-0.662464	1.259465	-0.041474
F	0.013096	0.005222	-1.221172
C	-2.565535	0.677453	-0.016041
C	-3.228543	0.316843	1.146293
C	-4.554777	-0.090444	1.155985
C	-5.296732	-0.125539	-0.023538
C	-4.664245	0.258227	-1.203383
C	-3.329127	0.644903	-1.168010
C	-0.782994	3.216923	1.027205
C	-1.307246	3.420788	-0.282101
C	-0.291918	3.091113	-1.221285
C	0.893318	2.741881	-0.488026
C	0.587498	2.824076	0.902292
C	-1.518131	3.411424	2.322661
H	-2.575385	3.144410	2.230283
H	-1.467684	4.455430	2.651497
H	-1.091889	2.789942	3.115053
C	-2.710029	3.841723	-0.604500
H	-3.416154	3.483285	0.150936
H	-3.032291	3.449573	-1.573257
H	-2.788224	4.933656	-0.641787
C	-0.374379	3.159651	-2.719568
H	-1.410568	3.156658	-3.064251
H	0.130720	2.306269	-3.182746
H	0.104106	4.071656	-3.093848
C	2.221987	2.458747	-1.127037
H	2.956536	2.113945	-0.394747
H	2.616025	3.368633	-1.593461
H	2.141361	1.695346	-1.908000
C	1.512596	2.565944	2.057488
H	1.620723	3.471415	2.663498
H	2.508483	2.276033	1.713846
H	1.145402	1.765949	2.706315
Al	0.665538	-1.264947	-0.044832
F	-0.010529	-0.010869	1.123845
C	2.567080	-0.681558	0.023036
C	3.355378	-0.631363	-1.115586
C	4.681066	-0.234513	-1.100256
C	5.291148	0.141536	0.096676
C	4.530458	0.088981	1.260526
C	3.202669	-0.331381	1.199760
C	0.322239	-3.080410	-1.257199
C	1.314026	-3.422587	-0.297459
C	0.757606	-3.234726	1.000998
C	-0.609535	-2.840254	0.847160
C	-0.880609	-2.739840	-0.548960
C	0.441234	-3.129683	-2.753783
H	1.485509	-3.124617	-3.073040
H	-0.029746	-4.035649	-3.151518
H	-0.050680	-2.269171	-3.218019
C	2.724453	-3.840111	-0.589428
H	3.067646	-3.445917	-1.550125
H	3.412988	-3.481669	0.182121
H	2.805668	-4.931823	-0.626746
C	1.460271	-3.445895	2.311775
H	2.519344	-3.177523	2.249095
H	1.014140	-2.834462	3.101056
H	1.402020	-4.494015	2.625954
C	-1.563482	-2.598035	1.982106
H	-2.553316	-2.314086	1.616632
H	-1.678694	-3.509073	2.578348
H	-1.218239	-1.800460	2.645784
C	-2.192218	-2.444228	-1.216999
H	-2.572912	-3.344571	-1.712165
H	-2.945873	-2.114804	-0.497082
H	-2.091560	-1.664538	-1.979359
F	2.814932	-0.957893	-2.306697
F	5.382915	-0.196359	-2.232568
F	-2.582905	0.349524	2.325705
F	-5.129640	-0.453298	2.302613
C	-6.732472	-0.573425	0.066626
C	6.732013	0.577893	0.039810
F	-6.807813	-1.820719	0.546899
F	-7.348139	-0.554106	-1.114757
F	-7.421376	0.215539	0.899779
F	-5.299158	0.256258	-2.372828
F	-2.759994	0.983444	-2.343323
F	6.870206	1.642034	-0.760416
F	7.500831	-0.397388	-0.459060
F	7.214648	0.904108	1.238177
F	5.032152	0.434580	2.443835
F	2.530127	-0.381545	2.364225

4b'_4

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Al	2.045971	-1.293939	-0.282825
F	2.118805	-0.104435	1.142560
C	0.094809	-1.641376	-0.158985
C	-0.845644	-1.360103	-1.137026
C	-2.206005	-1.529885	-0.933365
C	-2.685572	-2.038965	0.274637
C	-1.762746	-2.335713	1.272490
C	-0.408738	-2.133302	1.030340
C	2.693460	-2.928979	-1.685089
C	2.443268	-3.539362	-0.422707
C	3.290551	-2.929240	0.539616
C	4.115158	-1.970378	-0.141122
C	3.749299	-1.980136	-1.521537
C	1.974757	-3.235804	-2.968306
H	0.892696	-3.309248	-2.815779
H	2.313941	-4.186041	-3.395104
H	2.146100	-2.452621	-3.711697
C	1.412124	-4.596885	-0.165717
H	0.539874	-4.462361	-0.813086

H	1.064587	-4.574115	0.870453
H	1.822265	-5.593439	-0.362510
C	3.402745	-3.246951	2.003102
H	2.543057	-3.819873	2.354900
H	3.458397	-2.333113	2.603772
H	4.306921	-3.833190	2.203264
C	5.215128	-1.196895	0.527951
H	5.845224	-0.685157	-0.202614
H	5.854391	-1.873459	1.104898
H	4.823639	-0.444109	1.221785
C	4.350734	-1.161579	-2.629884
H	4.601730	-1.802289	-3.480612
H	5.272855	-0.674781	-2.302454
H	3.668958	-0.382443	-2.986854
Al	1.724455	1.482733	0.279968
F	2.079663	0.342238	-1.141634
C	-0.258734	1.452900	0.144441
C	-0.834363	1.869800	-1.045859
C	-2.202780	1.939677	-1.241629
C	-3.080904	1.595403	-0.214732
C	-2.533912	1.148905	0.985558
C	-1.149413	1.095078	1.140089
C	2.612936	3.343842	-0.531920
C	1.639356	3.770036	0.409968
C	1.986475	3.230399	1.681644
C	3.218903	2.521154	1.545151
C	3.605657	2.581461	0.171949
C	2.685905	3.670572	-1.995940
H	1.734471	4.054299	-2.368157
H	3.455444	4.427684	-2.185401
H	2.937852	2.783985	-2.587129
C	0.420703	4.596194	0.126513
H	0.114239	4.512151	-0.919579
H	-0.424151	4.280702	0.747205
H	0.612861	5.653703	0.337949
C	1.200384	3.391142	2.951556
H	0.124562	3.293313	2.772928
H	1.478888	2.630756	3.686304
H	1.372583	4.374841	3.402249
C	3.954383	1.848906	2.670676
H	4.961134	1.555859	2.362257
H	4.056324	2.532747	3.518777
H	3.437773	0.950514	3.024464
C	4.853827	2.047099	-0.469959
H	5.344970	2.833715	-1.052405
H	5.566448	1.691814	0.277521
H	4.640400	1.217545	-1.153724
F	-0.037133	2.250396	-2.064295
F	-2.685199	2.358683	-2.410186
F	-0.447699	-0.846562	-2.314670
F	-3.069927	-1.171646	-1.883961
C	-4.174406	-2.189354	0.439671
C	-4.556957	1.760643	-0.474559
F	-4.773125	-0.991650	0.438741
F	-4.503033	-2.805643	1.574132
F	-4.693997	-2.895784	-0.571237
F	-2.134891	-2.806927	2.458975
F	0.443631	-2.430121	2.032531
F	-4.974720	0.930469	-1.433718
F	-4.812203	3.010101	-0.892125
F	-5.294488	1.549479	0.614539
F	-3.300686	0.749121	1.997529
F	-0.682365	0.649890	2.322086

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C	2.774500	-1.150744	0.050836
C	3.373494	0.000034	-0.535668
C	2.774667	1.151164	0.050397
C	1.813060	-0.711431	1.006398
C	1.813153	0.712370	1.006110
C	0.989208	-1.620132	1.873721
H	0.546313	-2.440269	1.299332
H	1.606338	-2.068010	2.661008
H	0.172182	-1.085919	2.364526
C	0.989147	1.621465	1.872900
H	0.172348	1.087319	2.364160
H	1.606213	2.070079	2.659815
H	0.545924	2.441076	1.298006
C	3.123722	2.582172	-0.240013
H	2.263710	3.240255	-0.085983
H	3.927992	2.930638	0.418284
H	3.461305	2.714044	-1.271796
C	4.470017	-0.000259	-1.561285
H	4.417643	0.882369	-2.204794
H	5.454915	-0.000949	-1.080568
H	4.416674	-0.882427	-2.205354
C	3.123264	-2.581941	-0.238950
H	3.461911	-2.714123	-1.270343
H	3.926698	-2.930617	0.420260
H	2.262840	-3.239673	-0.085722
Al	1.133165	0.000314	-1.096186
C	-2.469823	-0.000599	-1.493935
C	-2.374907	-1.203333	-0.807206
C	-2.195197	-1.203879	0.569842
C	-2.113638	0.000050	1.256755
C	-2.196185	1.203664	0.569394
C	-2.376041	1.202475	-0.807628
F	-2.589988	-0.000931	-2.814271
F	-2.423022	2.350804	-1.470721
F	-2.096544	2.352958	1.229128
F	-1.939938	0.000388	2.577921
F	-2.094689	-2.352861	1.229990
F	-2.420795	-2.351950	-1.469873

4c_Int2

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C	1.714032	-0.817669	1.290513
C	2.759671	-1.046425	0.331673
C	3.223091	0.227299	-0.123165
C	1.518637	0.580739	1.402181
C	2.420958	1.235683	0.503364
C	0.489589	1.260041	2.255646
H	-0.371575	0.607926	2.430239
H	0.906183	1.531257	3.231846
H	0.120929	2.174880	1.783547
C	2.550916	2.723488	0.327787
H	1.573867	3.213497	0.357515
H	3.167228	3.156305	1.122824
H	3.017137	2.973520	-0.628347
C	4.318071	0.446510	-1.124430
H	4.215473	1.413568	-1.621899
H	5.298869	0.421115	-0.636993
H	4.304359	-0.322372	-1.900788
C	3.326502	-2.376032	-0.080688
H	3.624633	-2.371065	-1.132773
H	4.210593	-2.624609	0.516159
H	2.598537	-3.180173	0.052888
C	0.933281	-1.869107	2.024130
H	0.976709	-2.833538	1.513338
H	1.323439	-2.007158	3.038076
H	-0.122472	-1.592203	2.110512
Al	1.163021	-0.044443	-0.748913
C	-0.797055	-0.019887	-0.529393
C	-1.525024	-1.190900	-0.407957
C	-2.895635	-1.214020	-0.184603
C	-3.574243	-0.005546	-0.079052
C	-2.883310	1.195824	-0.188996
C	-1.513702	1.158302	-0.412490
F	1.475530	-0.144796	-2.386036
F	-0.864460	2.337113	-0.499021
F	-3.538809	2.349541	-0.078802
F	-4.885976	0.001682	0.135713
F	-3.562606	-2.360637	-0.070029
F	-0.885664	-2.373235	-0.493759

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C	3.230109	-0.879768	0.463553
C	2.946577	-0.481714	-0.884282
C	2.478919	0.864127	-0.853311
C	2.941973	0.226080	1.318870
C	2.467700	1.299016	0.507544
C	3.106934	0.248121	2.810635
H	2.939755	-0.740548	3.246946
H	4.117966	0.565997	3.088061
H	2.401777	0.938522	3.280865
C	2.062436	2.669179	0.968907
H	1.830127	2.679404	2.036636
H	2.871291	3.387811	0.797187
H	1.178304	3.022878	0.431876
C	2.055366	1.685917	-2.036099
H	1.143614	2.249790	-1.822770

H	2.839664	2.399009	-2.312581
H	1.855760	1.051829	-2.903017
C	3.125016	-1.316643	-2.120149
H	2.282834	-1.196204	-2.807819
H	4.037737	-1.030677	-2.653778
H	3.202043	-2.378659	-1.874805
C	3.789906	-2.204544	0.894782
H	3.456300	-3.015270	0.241932
H	4.885084	-2.187406	0.871426
H	3.484214	-2.454567	1.914005
Al	1.038250	-0.422323	0.240733
C	-1.104165	-0.294742	-0.393185
C	-1.959300	-1.390508	-0.180643
C	-3.270509	-1.215321	0.217238
C	-3.822911	0.060308	0.292931
C	-3.011284	1.159069	0.034422
C	-1.700805	0.977010	-0.364778
F	-0.134039	-0.470604	-1.539481
F	-0.910415	2.057539	-0.523571
F	-3.511152	2.390199	0.137387
F	-5.105561	0.225438	0.619693
F	-4.026968	-2.275272	0.499417
F	-1.427363	-2.620103	-0.162591

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Al	0.882564	1.121874	-0.013000
F	-0.003716	0.018052	1.171936
F	2.752316	0.134922	-2.363574
F	5.241470	-0.889643	-2.337988
F	6.491868	-1.365331	0.028406
F	5.249319	-0.770802	2.371114
F	2.780670	0.314752	2.349265
C	2.668777	0.257856	-0.007216
C	3.352349	-0.051205	-1.171482
C	4.630242	-0.594785	-1.191963
C	5.269375	-0.843994	0.016762
C	4.630661	-0.542526	1.214090
C	3.356092	0.008692	1.169157
C	1.437725	3.058328	-1.043935
C	1.896867	3.156845	0.301128
C	0.780341	3.000225	1.165582
C	-0.392006	2.857022	0.350328
C	0.018497	2.884841	-1.017096
C	2.297391	3.156712	-2.271239
H	3.287979	2.723301	-2.103009
H	2.439366	4.203113	-2.563186
H	1.852169	2.629802	-3.118644
C	3.326938	3.314196	0.725286
H	4.007783	2.836697	0.013548
H	3.503768	2.861328	1.705440
H	3.601501	4.372646	0.791190
C	0.777428	3.031449	2.667411
H	1.764398	2.799726	3.074429
H	0.072587	2.300418	3.075080
H	0.483318	4.020119	3.037304
C	-1.796934	2.840307	0.876615
H	-2.510911	2.531529	0.108497
H	-2.080776	3.844419	1.212517
H	-1.901291	2.163870	1.730253
C	-0.883030	2.759852	-2.211356
H	-1.240815	3.743363	-2.534589
H	-1.755324	2.138814	-1.990702
H	-0.363444	2.297469	-3.054478
Al	-0.882574	-1.121987	0.012995
F	0.003775	-0.018218	-1.171947
F	-2.752157	-0.134661	2.363552
F	-5.241252	0.890046	2.337966
F	-6.491702	1.365611	-0.028424
F	-5.249269	0.770814	-2.371125
F	-2.780693	-0.314905	-2.349270
C	-2.668733	-0.257863	0.007203
C	-3.352241	0.051350	1.171468
C	-4.630092	0.595030	1.191947
C	-5.269249	0.844180	-0.016778
C	-4.630594	0.542577	-1.214103
C	-3.356058	-0.008719	-1.169168
C	-1.437831	-3.058391	1.043953
C	-1.897002	-3.156844	-0.301105
C	-0.780464	-3.000344	-1.165563
C	0.391900	-2.857242	-0.350316
C	-0.018593	-2.884980	1.017110
C	-2.297494	-3.156720	2.271264
H	-3.288061	-2.723261	2.103034
H	-2.439519	-4.203111	2.563225
H	-1.852240	-2.629821	3.118659
C	-3.327096	-3.314002	-0.725248
H	-4.007870	-2.836409	-0.013503
H	-3.503879	-2.861110	-1.705400
H	-3.601800	-4.372415	-0.791146
C	-0.777558	-3.031582	-2.667392
H	-1.764509	-2.799780	-3.074410
H	-0.072657	-2.300612	-3.075066
H	-0.483529	-4.020279	-3.037278
C	1.796821	-2.840694	-0.876613
H	2.510838	-2.531985	-0.108507
H	2.080543	-3.844848	-1.212490
H	1.901243	-2.164299	-1.730274
C	0.882946	-2.760029	2.211364
H	1.240663	-3.743560	2.534613
H	1.755283	-2.139056	1.990699
H	0.363394	-2.297597	3.054480

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Al	1.218008	-1.415695	-0.194130
F	1.428528	-0.154512	1.152520
C	-0.754372	-1.582973	-0.095787
C	-1.622932	-1.247347	-1.121078
C	-3.004996	-1.291295	-0.992043
C	-3.557564	-1.701760	0.215226
C	-2.727654	-2.062986	1.269188
C	-1.353132	-1.991839	1.085176
C	1.708090	-3.197318	-1.500377
C	1.400127	-3.705488	-0.207291
C	2.296960	-3.119287	0.724182
C	3.210824	-2.285879	-0.006669
C	2.847289	-2.343397	-1.386303
C	0.960232	-3.507398	-2.765636
H	-0.123335	-3.461084	-2.611843
H	1.199329	-4.511595	-3.132764
H	1.207929	-2.792150	-3.554560
C	0.274618	-4.646574	0.099942
H	-0.588181	-4.451658	-0.545025
H	-0.056828	-4.550535	1.136876
H	0.583750	-5.685137	-0.061546
C	2.373807	-3.356695	2.205150
H	1.448687	-3.790805	2.588625
H	2.547693	-2.420626	2.746093
H	3.196329	-4.039478	2.447493
C	4.383832	-1.588091	0.619813
H	5.065461	-1.196007	-0.138125
H	4.947664	-2.287275	1.246378
H	4.073203	-0.753199	1.257939
C	3.526364	-1.654645	-2.537240
H	3.690676	-2.360079	-3.357309
H	4.503153	-1.264524	-2.239824
H	2.935994	-0.818684	-2.927272
Al	1.216210	1.416617	0.193762
F	1.428624	0.155788	-1.152857
C	-0.756440	1.581166	0.095088
C	-1.355936	1.989126	-1.085883
C	-2.730536	2.058966	-1.269436
C	-3.559854	1.697355	-0.215079
C	-3.006586	1.287757	0.992110
C	-1.624381	1.245077	1.120680
C	2.293144	3.121310	-0.724095
C	1.394091	3.707136	0.205464
C	1.700881	3.200801	1.499499
C	2.841418	2.348398	1.388059
C	3.207219	2.290033	0.009000
C	2.371764	3.357427	-2.205170
H	1.445798	3.787921	-2.590696
H	3.192357	4.042745	-2.446876
H	2.549775	2.421365	-2.744781
C	0.267847	4.646501	-0.104294
H	-0.062094	4.549056	-1.141569
H	-0.595565	4.451247	0.539753
H	0.575557	5.685587	0.056566
C	0.950460	3.510898	2.763222
H	-0.132783	3.461902	2.607940
H	1.198684	2.797354	3.553520
H	1.186713	4.516165	3.129258

C	3.519580	1.661671	2.540746
H	4.496229	1.270229	2.244653
H	3.683980	2.368743	3.359393
H	2.928483	0.826911	2.932237
C	4.382750	1.594111	-0.614845
H	4.947992	2.294704	-1.238580
H	5.062331	1.201433	0.144591
H	4.074807	0.759916	-1.255178
F	-0.579546	2.332609	-2.133527
F	-3.258908	2.445260	-2.428211
F	-1.130467	-0.808205	-2.293987
F	-3.804896	-0.878393	-1.975931
F	-3.255186	-2.450170	2.428033
F	-0.576137	-2.335032	2.132488
F	-3.805701	0.874471	1.976454
F	-1.131224	0.806815	2.293666
F	-4.879273	1.709967	-0.368327
F	-4.876939	-1.715598	0.368734

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C	-3.330974	-0.751688	-0.836380
C	-2.700731	-1.142786	0.378762
C	-2.359802	0.036706	1.098815
C	-3.371646	0.672647	-0.870866
C	-2.769585	1.159177	0.325978
C	-3.981255	1.509811	-1.958555
H	-3.921752	1.010225	-2.929509
H	-5.039368	1.709448	-1.754073
H	-3.475892	2.474803	-2.054503
C	-2.612433	2.599699	0.721055
H	-2.619887	3.255563	-0.153579
H	-3.426758	2.919281	1.381216
H	-1.669334	2.767660	1.249527
C	-1.749907	0.068674	2.470412
H	-2.494200	-0.211692	3.224817
H	-0.907950	-0.622860	2.557773
H	-1.383743	1.067207	2.719552
C	-2.460757	-2.544421	0.860052
H	-1.505039	-2.622292	1.386920
H	-3.249172	-2.862527	1.552154
H	-2.442494	-3.256438	0.030480
C	-3.887158	-1.674927	-1.881920
H	-3.337234	-2.619532	-1.915964
H	-4.937915	-1.910916	-1.678339
H	-3.836715	-1.229309	-2.879330
Al	-1.154323	0.027893	-0.889345
C	1.929272	-0.985391	0.818041
C	3.825719	-0.941162	-0.619478
C	3.819295	0.448061	-0.606834
C	2.849327	1.116286	0.129346
C	1.904155	0.401430	0.852110
F	0.992544	-1.655951	1.495598
F	0.964416	1.051713	1.536713
F	2.822536	2.442889	0.139511
F	4.725755	1.138172	-1.291791
F	4.764190	-1.562794	-1.331244
C	2.885831	-1.672553	0.089542
H	2.892574	-2.754867	0.064783

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C	-2.801849	1.063268	0.245337
C	-3.149766	-0.270130	-0.131648
C	-2.272503	-1.166732	0.559522
C	-1.748875	0.983857	1.218552
C	-1.435419	-0.383369	1.416952
C	-1.060545	2.135116	1.892877
H	-1.280002	3.082735	1.393969
H	-1.385506	2.228298	2.934594
H	0.026861	2.003455	1.896249
C	-0.360816	-0.908066	2.321844
H	0.467241	-0.196906	2.404440
H	-0.749575	-1.087058	3.330391
H	0.049234	-1.850441	1.949028
C	-2.288728	-2.667983	0.481793
H	-2.935881	-3.089421	1.258187
H	-2.659609	-3.014799	-0.486087
H	-1.286681	-3.081588	0.617082
C	-4.218691	-0.632996	-1.119546
H	-4.124310	-1.671979	-1.442758
H	-5.212615	-0.509142	-0.675667
H	-4.163126	-0.004379	-2.012339
C	-3.492290	2.301455	-0.253824
H	-3.733375	2.217247	-1.317523
H	-4.429523	2.469136	0.287913
H	-2.871633	3.191520	-0.123445
Al	-1.110359	0.137963	-0.774399
C	0.847380	0.256364	-0.567875
C	2.995580	1.349613	-0.298661
C	3.629716	0.124177	-0.120101
C	2.878128	-1.040919	-0.163826
C	1.510840	-0.944130	-0.388495
F	-1.454543	0.178611	-2.410394
F	0.805548	-2.100073	-0.414178
F	3.469431	-2.220906	0.008494
F	4.941701	0.063583	0.093824
F	3.744238	2.455584	-0.248850
C	1.629524	1.420725	-0.518428
H	1.195670	2.407090	-0.653753

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C	3.224180	-0.899007	0.356198
C	2.822921	-0.492554	-0.955553
C	2.313373	0.834582	-0.868410
C	2.973234	0.188519	1.247762
C	2.403887	1.254951	0.494722
C	3.255049	0.195796	2.722074
H	3.216982	-0.813951	3.140032
H	4.251013	0.602323	2.930200
H	2.528412	0.804340	3.267429
C	1.989603	2.599353	1.020588
H	1.871109	2.580371	2.106775
H	2.742995	3.357941	0.782050
H	1.038305	2.920069	0.587975
C	1.786274	1.633112	-2.026105
H	2.588352	1.855048	-2.738161
H	1.001319	1.087705	-2.559250
H	1.359931	2.580329	-1.689613
C	2.921609	-1.288395	-2.224150
H	2.043020	-1.128067	-2.856314
H	3.806302	-0.993489	-2.799539
H	2.997290	-2.360315	-2.024163
C	3.863313	-2.207800	0.721029
H	3.564510	-3.004719	0.035042
H	4.955421	-2.129309	0.682629
H	3.589742	-2.521499	1.732087
Al	0.996552	-0.518006	0.313802
C	-1.196454	-0.604527	-0.245888
C	-3.422080	-1.371690	0.267994
C	-3.915184	-0.070740	0.265096
C	-3.032081	0.966915	-0.011661
C	-1.715795	0.696281	-0.330939
F	-0.171182	-0.890500	-1.357711
F	-0.866407	1.723837	-0.531911
F	-3.465717	2.226178	0.005787
F	-5.196385	0.184953	0.537703
F	-4.275098	-2.363063	0.542034
C	-2.100140	-1.659293	-0.010230
H	-1.767047	-2.688374	0.025109

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Al	-0.84169900	1.12981600	-0.21482700
F	0.13033000	-0.11118200	-1.20429100
C	-2.61650700	0.27810800	-0.38721800
C	-3.34920400	-0.06170800	0.73516700
C	-4.59227300	-0.68669600	0.67682400
C	-5.14897500	-0.96271700	-0.56324500
C	-4.45207900	-0.60479400	-1.71470600
C	-3.21097400	0.00046900	-1.62990500
C	-1.36615300	3.17823400	0.58100800
C	-1.76250200	3.16408100	-0.78449300
C	-0.61741600	2.87692800	-1.57470500
C	0.51599800	2.77928400	-0.69553800
C	0.04777500	2.97277700	0.63819400
C	-2.27263300	3.40774200	1.75631400
H	-3.23184000	2.89545400	1.62978800

H	-2.48160500	4.47504900	1.89120200
H	-1.82270000	3.03570100	2.68079500
C	-3.17016000	3.35606300	-1.26287000
H	-3.88274400	2.82225100	-0.62543000
H	-3.30668400	2.99070100	-2.28397700
H	-3.43916200	4.41811000	-1.24850200
C	-0.53767700	2.76239900	-3.07106600
H	-1.52625100	2.62272900	-3.51663200
H	0.08962500	1.91784900	-3.37425300
H	-0.10338400	3.66747900	-3.51060500
C	1.93340000	2.62130400	-1.16584100
H	2.61999400	2.45324500	-0.33223900
H	2.25737000	3.52546300	-1.69386900
H	2.03748500	1.77779800	-1.85636400
C	0.86642000	3.00668700	1.89686100
H	0.79663500	3.99397800	2.36544400
H	1.92001800	2.80597300	1.69293000
H	0.52127700	2.26717900	2.62695700
Al	0.85475500	-1.14511100	0.14675600
F	-0.10930700	0.10307200	1.12933700
C	2.62010200	-0.27926000	0.35605300
C	3.53108900	-0.28143500	-0.68498500
C	4.78750900	0.30587100	-0.60849200
C	5.16284400	0.93415400	0.57174900
C	4.27709200	0.94632000	1.64417500
C	3.03077500	0.34781400	1.54232400
C	0.90549200	-3.13810100	-0.82354600
C	1.82154200	-3.21546000	0.26016800
C	1.10648000	-2.95970700	1.46367400
C	-0.27465400	-2.78749500	1.13579000
C	-0.40290800	-2.89505800	-0.28006900
C	1.19640800	-3.36056200	-2.28034700
H	2.25282400	-3.20047900	-2.50598700
H	0.93688500	-4.38288100	-2.57802000
H	0.61757700	-2.67647100	-2.90865800
C	3.29950500	-3.44818900	0.16225500
H	3.68969700	-3.13674300	-0.81055300
H	3.84040400	-2.88745700	0.93116600
H	3.53514000	-4.50991300	0.29495800
C	1.69368400	-2.89876200	2.84493500
H	2.66137900	-2.38562100	2.84954300
H	1.02942500	-2.36482200	3.53104300
H	1.85210100	-3.90309400	3.25351100
C	-1.37663300	-2.56149700	2.13163900
H	-2.34157700	-2.43664600	1.63484900
H	-1.45816600	-3.42007400	2.80641700
H	-1.20749600	-1.66791200	2.73879700
C	-1.66685300	-2.90364800	-1.08867700
H	-1.88888500	-3.92208700	-1.42759200
H	-2.52221200	-2.54649700	-0.50999000
H	-1.58298700	-2.26855600	-1.97541100
H	2.37662100	0.39820800	2.40875900
H	-2.70528100	0.24010200	-2.56263900
F	3.20055900	-0.86038100	-1.86162900
F	5.62622600	0.28504900	-1.64256000
F	6.35948300	1.50800000	0.67030500
F	-2.86559900	0.20603000	1.96678200
F	-5.24687600	-1.01905300	1.78801900
F	-6.33996700	-1.55051000	-0.64505000
F	-5.01613600	-0.87212000	-2.89699700
F	4.65705900	1.56244600	2.76891800

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Al	1.183077	-1.426470	-0.084726
F	1.423360	-0.053829	1.165550
C	-0.770578	-1.577117	0.139632
C	-1.639296	-1.437847	-0.926786
C	-3.022455	-1.448977	-0.786453
C	-3.572884	-1.637763	0.472680
C	-2.726589	-1.802652	1.564549
C	-1.351612	-1.771739	1.403752
C	1.676061	-3.335430	-1.221776
C	1.353030	-3.731096	0.104646
C	2.236351	-3.064426	0.993066
C	3.161743	-2.297380	0.205254
C	2.814745	-2.474819	-1.168319
C	0.949181	-3.765520	-2.463926
H	-0.136373	-3.720418	-2.328380
H	1.207717	-4.794621	-2.737559
H	1.198234	-3.119515	-3.310161
C	0.217543	-4.639689	0.466766
H	-0.671912	-4.417737	-0.131767
H	-0.063078	-4.540526	1.518506
H	0.489854	-5.685958	0.288477
C	2.284436	-3.161913	2.491818
H	1.346257	-3.547776	2.899418
H	2.469635	-2.183531	2.947759
H	3.086380	-3.834513	2.817342
C	4.327567	-1.544607	0.779627
H	5.004986	-1.202066	-0.005654
H	4.899691	-2.189818	1.454847
H	4.008149	-0.668022	1.354271
C	3.511599	-1.896641	-2.368183
H	3.716110	-2.682232	-3.102014
H	4.469312	-1.449572	-2.090182
H	2.912464	-1.124599	-2.862471
Al	1.184931	1.425594	0.084298
F	1.423495	0.052578	-1.165980
C	-0.768513	1.578798	-0.139954
C	-1.349649	1.773747	-1.403978
C	-2.724624	1.805621	-1.564513
C	-3.570807	1.641308	-0.472465
C	-3.020287	1.452153	0.786568
C	-1.637109	1.440163	0.926644
C	2.241772	3.061369	-0.993034
C	1.358563	3.729813	-0.105803
C	1.679724	3.334335	1.221128
C	2.817132	2.471982	1.169213
C	3.165255	2.293361	-0.203919
C	2.291464	3.158095	-2.491784
H	1.353620	3.543425	-2.900666
H	3.093551	3.830768	-2.816800
H	2.477449	2.179504	-2.946939
C	0.224729	4.639778	-0.469662
H	-0.055056	4.540168	-1.521585
H	-0.665600	4.419605	0.128219
H	0.498391	5.685800	-0.292001
C	0.952198	3.765856	2.462395
H	-0.133265	3.723715	2.325189
H	1.198240	3.118809	3.308719
H	1.213080	4.794139	2.736884
C	3.511771	1.893203	2.370064
H	4.468567	1.443509	2.093153
H	3.717691	2.678949	3.103341
H	2.910398	1.123070	2.864609
C	4.330607	1.538618	-0.776664
H	4.904747	2.182816	-1.451142
H	5.006368	1.194995	0.009568
H	4.010543	0.662528	-1.351689
F	-3.278164	1.977001	-2.768548
F	-1.152125	-1.228399	-2.168340
F	-3.821064	-1.220290	-1.828678
F	-3.280008	-1.973731	2.768687
F	-3.818884	1.223927	1.828900
F	-1.149810	1.230233	2.168064
F	-4.891566	1.622768	-0.629716
F	-4.893601	-1.618529	0.630181
H	-0.739746	1.870150	-2.298750
H	-0.741622	-1.868702	2.298406

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C	-2.706498	-1.051436	-0.405842
C	-1.697094	-1.066177	0.599715
C	-1.660291	0.223019	1.202789
C	-3.298979	0.242743	-0.419895
C	-2.648024	1.032027	0.569766
C	-4.433708	0.685491	-1.297700
H	-4.430818	0.155764	-2.254465
H	-5.399350	0.493074	-0.816344
H	-4.380091	1.756338	-1.513092
C	-2.971273	2.453131	0.930130
H	-3.358601	3.008886	0.071621
H	-3.729843	2.494398	1.720439
H	-2.086300	2.982120	1.295398
C	-0.778884	0.673593	2.332604
H	-0.346624	1.661027	2.141603
H	-1.349613	0.740317	3.265984
H	0.049741	-0.017261	2.504602
C	-0.864578	-2.263367	0.960731
H	-0.025177	-1.996995	1.607122
H	-1.467120	-3.006203	1.496010
H	-0.451741	-2.755685	0.074003

C	-3.103190	-2.221820	-1.258269
H	-2.255842	-2.891153	-1.433175
H	-3.892880	-2.809190	-0.775426
H	-3.479942	-1.901721	-2.233821
Al	-1.078325	0.468884	-1.031701
C	2.258329	-0.635861	0.933284
C	2.309676	-1.486142	-0.163295
C	2.562294	0.380584	-1.620551
C	2.500886	1.251874	-0.541050
C	2.344213	0.736661	0.738890
F	2.109767	-1.124897	2.165919
F	2.273583	1.556971	1.781243
F	2.555170	2.566350	-0.724175
F	2.681086	0.896430	-2.840571
F	2.206413	-2.798208	0.048724
C	2.468838	-0.991084	-1.447777
H	2.497941	-1.658428	-2.299806

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C	-2.374611	1.126901	0.500068
C	-3.075695	0.042000	-0.118686
C	-2.489264	-1.177607	0.342014
C	-1.411726	0.568062	1.401144
C	-1.470621	-0.842961	1.298131
C	-0.450930	1.350723	2.245589
H	-0.181657	2.296637	1.767787
H	-0.884906	1.580551	3.224902
H	0.474509	0.791537	2.413036
C	-0.588700	-1.811463	2.031130
H	0.425240	-1.415218	2.146585
H	-0.981014	-2.015873	3.033052
H	-0.507337	-2.763156	1.501084
C	-2.927493	-2.557590	-0.061177
H	-2.128281	-3.289241	0.081806
H	-3.787031	-2.883272	0.534626
H	-3.220787	-2.588570	-1.114294
C	-4.187931	0.143229	-1.119815
H	-4.070591	-0.594432	-1.917650
H	-5.157868	-0.025466	-0.639153
H	-4.212917	1.129326	-1.588860
C	-2.646017	2.594395	0.315386
H	-3.147752	2.791102	-0.635193
H	-3.287612	2.975738	1.116811
H	-1.718402	3.173243	0.324971
Al	-0.998068	-0.032313	-0.751119
C	0.947317	0.174777	-0.536765
C	1.560018	1.413713	-0.430636
C	3.706276	0.479780	-0.096488
C	3.161540	-0.795648	-0.186740
C	1.794735	-0.912121	-0.405790
F	-1.317586	-0.166535	-2.385533
F	1.281866	-2.154489	-0.479633
F	3.937563	-1.872826	-0.064630
F	5.018008	0.593651	0.113917
F	0.773376	2.511168	-0.531518
C	2.915383	1.613099	-0.213671
H	3.348562	2.602722	-0.140551

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C	3.160182	-0.682973	0.342834
C	2.732690	-0.281863	-0.962746
C	2.115463	0.996777	-0.849932
C	2.810453	0.357748	1.257211
C	2.158051	1.390150	0.522760
C	3.081121	0.353360	2.733679
H	3.093078	-0.664037	3.134481
H	4.052668	0.808199	2.956486
H	2.319455	0.913449	3.282903
C	1.618955	2.679370	1.073819
H	1.485992	2.623060	2.157012
H	2.304866	3.507835	0.866228
H	0.649435	2.924080	0.631715
C	1.536819	1.777340	-1.995214
H	1.062032	2.696301	-1.645523
H	2.322026	2.050654	-2.708192
H	0.779608	1.196346	-2.530356
C	2.904078	-1.036677	-2.248687
H	2.010782	-0.950615	-2.874851
H	3.752269	-0.642906	-2.819887
H	3.086496	-2.099662	-2.071758
C	3.901892	-1.943289	0.682660
H	3.652270	-2.753503	-0.007379
H	4.984213	-1.781939	0.628902
H	3.667936	-2.286537	1.693929
Al	0.914811	-0.494375	0.297024
C	-1.257399	-0.586514	-0.260989
C	-2.051197	-1.698353	0.069401
C	-3.984025	-0.339908	0.396239
C	-3.253728	0.782046	0.023185
C	-1.930278	0.640358	-0.354123
F	-0.275568	-0.821635	-1.405462
F	-1.212685	1.742082	-0.641309
F	-3.825799	1.986949	0.002443
F	-5.274488	-0.195837	0.716696
F	-1.432816	-2.886078	0.156371
C	-3.374661	-1.587528	0.442829
H	-3.933967	-2.463431	0.748764

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Al	-0.885330	-1.162513	0.043874
F	0.078671	-0.101486	1.213112
C	-2.662832	-0.298240	0.178669
C	-3.321192	0.240185	-0.914734
C	-4.556197	0.876119	-0.836571
C	-5.182909	0.952157	0.400773
C	-4.597542	0.408867	1.535449
C	-3.359511	-0.194238	1.374361
C	-1.356272	-3.030838	-1.096331
C	-1.833468	-3.222513	0.231435
C	-0.731668	-3.095176	1.120260
C	0.451175	-2.887874	0.332507
C	0.062318	-2.850913	-1.038290
C	-2.187338	-3.037597	-2.347644
H	-3.151913	-2.543226	-2.193829
H	-2.388682	-4.060792	-2.684229
H	-1.677662	-2.511901	-3.159859
C	-3.265924	-3.437346	0.618295
H	-3.943220	-2.932242	-0.077371
H	-3.470478	-3.049029	1.620057
H	-3.515420	-4.504131	0.613092
C	-0.744039	-3.227287	2.616361
H	-1.742852	-3.058618	3.024715
H	-0.069901	-2.501261	3.081563
H	-0.416954	-4.227447	2.922761
C	1.839023	-2.828363	0.902013
H	2.580300	-2.588253	0.135614
H	2.108010	-3.796652	1.339157
H	1.920878	-2.074189	1.691841
C	0.955678	-2.668566	-2.232115
H	0.883254	-3.537246	-2.894917
H	2.000482	-2.565020	-1.929716
H	0.693206	-1.777586	-2.809366
Al	0.853689	1.099538	0.035519
F	-0.113714	0.041975	-1.122663
C	2.624995	0.248815	-0.217648
C	3.481481	0.010010	0.844856
C	4.743112	-0.553868	0.717391
C	5.180479	-0.898291	-0.556450
C	4.387975	-0.674486	-1.671883
C	3.141190	-0.097860	-1.458201
C	0.881708	2.879072	1.358973
C	1.852689	3.125714	0.350971
C	1.195106	3.106223	-0.911802
C	-0.203951	2.912794	-0.683311
C	-0.400819	2.769821	0.721567
C	1.100509	2.811775	2.843514
H	2.147538	2.616943	3.085641
H	0.811755	3.753577	3.323926
H	0.503316	2.012826	3.294146
C	3.327511	3.296590	0.560903
H	3.660705	2.800655	1.477068
H	3.897734	2.871984	-0.271314
H	3.589707	4.357424	0.639085
C	1.844891	3.285732	-2.253980
H	2.834750	2.819681	-2.287174

H	1.243601	2.831549	-3.046404
H	1.969449	4.347766	-2.493787
C	-1.253011	2.886466	-1.758304
H	-2.247562	2.712037	-1.340687
H	-1.277317	3.845441	-2.286409
H	-1.065848	2.099178	-2.493815
C	-1.698382	2.638027	1.464775
H	-1.902949	3.555202	2.028954
H	-2.538195	2.466833	0.786721
H	-1.672178	1.808076	2.178479
H	4.738451	-0.932194	-2.663707
H	-5.089663	0.467976	2.498233
F	3.079318	0.322090	2.093620
F	5.519347	-0.766583	1.780895
F	6.390398	-1.443192	-0.686234
F	-2.760197	0.164165	-2.134958
F	-5.130260	1.399046	-1.921301
F	-6.370531	1.553492	0.475965
F	-2.775043	-0.705326	2.483956
F	2.383155	0.140469	-2.550773

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Al	1.061044	-1.427575	-0.063962
F	1.283176	-0.049766	1.162035
C	-0.906606	-1.585134	0.035433
C	-1.772761	-1.342096	-1.018109
C	-3.156110	-1.381355	-0.898226
C	-3.707257	-1.680410	0.341602
C	-2.902519	-1.947726	1.438148
C	-1.531084	-1.885812	1.238142
C	1.553640	-3.332465	-1.198928
C	1.243907	-3.716449	0.135224
C	2.138525	-3.044277	1.008466
C	3.052274	-2.281945	0.204083
C	2.690158	-2.469079	-1.164592
C	0.805084	-3.759722	-2.429053
H	-0.278331	-3.691744	-2.281659
H	1.037798	-4.796534	-2.696321
H	1.057810	-3.126577	-3.283858
C	0.116766	-4.623471	0.526825
H	-0.748240	-4.480229	-0.128633
H	-0.210274	-4.435970	1.552431
H	0.421024	-5.673536	0.454057
C	2.212919	-3.140896	2.505242
H	1.286445	-3.536108	2.925824
H	2.386212	-2.157844	2.955421
H	3.034456	-3.798091	2.813175
C	4.224606	-1.528212	0.763362
H	4.905264	-1.206103	-0.027720
H	4.789984	-2.166168	1.451033
H	3.912897	-0.638740	1.322294
C	3.369225	-1.889504	-2.374227
H	3.533600	-2.667483	-3.125881
H	4.345987	-1.473405	-2.114233
H	2.778704	-1.093010	-2.839331
Al	1.062304	1.427129	0.063436
F	1.282986	0.049006	-1.162546
C	-0.905362	1.585313	-0.035819
C	-1.529927	1.885967	-1.238464
C	-2.901384	1.948689	-1.438180
C	-3.706023	1.682187	-0.341378
C	-3.154765	1.383113	0.898416
C	-1.771430	1.343117	1.018003
C	2.142023	3.042103	-1.008408
C	1.246280	3.715599	-0.137290
C	1.553618	3.332762	1.197738
C	2.689764	2.468853	1.166123
C	3.054149	2.280166	-0.201755
C	2.218540	3.137333	-2.505166
H	1.290049	3.525374	-2.928010
H	3.036045	3.799765	-2.812587
H	2.399467	2.154836	-2.953521
C	0.120572	4.623043	-0.531997
H	-0.205408	4.433913	-1.557636
H	-0.745388	4.482095	0.122684
H	0.425944	5.672898	-0.460953
C	0.803562	3.761360	2.426454
H	-0.279698	3.698047	2.275981
H	1.051329	3.125890	3.281004
H	1.039872	4.796790	2.695919
C	3.366104	1.889933	2.377588
H	4.341534	1.469687	2.119338
H	3.532710	2.669216	3.127418
H	2.772462	1.096689	2.844257
C	4.227313	1.525532	-0.758119
H	4.795382	2.163293	-1.443746
H	4.905313	1.202260	0.034746
H	3.916357	0.636664	-1.318424
F	-0.737836	2.130452	-2.309147
F	-1.274433	-1.011919	-2.223077
F	-3.946831	-1.073697	-1.929125
F	-0.738871	-2.131354	2.308463
F	-3.945459	1.076205	1.929564
F	-1.272966	1.012967	2.222923
F	-5.033546	1.684624	-0.458431
F	-5.034749	-1.682075	0.459003
H	-3.333919	2.161305	-2.407654
H	-3.334943	-2.160478	2.407641

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C	-3.298887	-0.242434	-0.420085
C	-2.648213	-1.031826	0.569669
C	-1.660411	-0.222988	1.202811
C	-2.706170	1.051642	-0.405965
C	-1.696905	1.066204	0.599734
C	-3.102588	2.222122	-1.258393
H	-3.478257	1.902204	-2.234425
H	-3.892991	2.808988	-0.776108
H	-2.255355	2.891865	-1.432264
C	-0.864275	2.263230	0.961036
H	-0.451312	2.755697	0.074450
H	-1.466772	3.006016	1.496436
H	-0.024954	1.996619	1.607432
C	-0.779159	-0.673784	2.332663
H	0.049418	0.017082	2.504805
H	-1.349971	-0.740712	3.265969
H	-0.346849	-1.661161	2.141449
C	-2.971850	-2.452849	0.930035
H	-2.086948	-2.982289	1.294837
H	-3.730054	-2.493874	1.720711
H	-3.359857	-3.008313	0.071646
C	-4.433729	-0.684957	-1.297851
H	-5.399253	-0.493933	-0.815703
H	-4.431772	-0.153942	-2.253898
H	-4.379405	-1.755479	-1.514710
Al	-1.078265	-0.468937	-1.031671
C	2.344012	-0.736969	0.738741
C	2.500690	-1.251932	-0.541312
C	2.562230	-0.380436	-1.620602
C	2.309849	1.486026	-0.162944
C	2.258330	0.635507	0.933456
F	2.273252	-1.557512	1.780883
F	2.109951	1.124239	2.166221
F	2.206833	2.798068	0.049375
F	2.681012	-0.895960	-2.840756
F	2.554772	-2.566388	-0.724653
C	2.468948	0.991224	-1.447509
H	2.498175	1.658708	-2.299423

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0 1

C	-2.187010	1.235948	0.498416
C	-2.986944	0.228737	-0.132479
C	-2.526383	-1.045723	0.323558
C	-1.289367	0.579745	1.400755
C	-1.485411	-0.818336	1.287506
C	-0.262907	1.258000	2.258203
H	0.106619	2.173364	1.787881
H	-0.682238	1.527375	3.233810
H	0.598372	0.606168	2.433262
C	-0.707816	-1.870588	2.023290
H	0.347573	-1.593696	2.113456
H	-1.102153	-2.009567	3.035544
H	-0.748905	-2.834332	1.511080
C	-3.092248	-2.374457	-0.092908
H	-2.366450	-3.179555	0.046551
H	-3.981529	-2.621723	0.496810
H	-3.381913	-2.369260	-1.147404
C	-4.077401	0.448626	-1.138566
H	-4.057925	-0.317899	-1.917156
H	-5.060704	0.419651	-0.656323
H	-3.974345	1.417351	-1.632692

C	-2.312675	2.724080	0.322421
H	-2.920942	3.160288	1.121833
H	-1.333304	3.209925	0.343599
H	-2.785524	2.974802	-0.630270
Al	-0.924853	-0.044654	-0.751829
C	1.032498	-0.019909	-0.519255
C	1.746415	1.159193	-0.395974
C	3.115059	1.182924	-0.160516
C	3.127326	-1.200719	-0.155695
C	1.757772	-1.191749	-0.391116
F	-1.234180	-0.144914	-2.389901
F	1.115950	-2.374596	-0.482818
F	3.771089	-2.365282	-0.038732
F	3.747036	2.354499	-0.048411
F	1.094377	2.338469	-0.487927
C	3.820693	-0.005202	-0.040537
H	4.888414	0.000608	0.141276

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0 1

C	2.975727	-0.916411	0.407555
C	2.658935	-0.514181	-0.931804
C	2.222430	0.841791	-0.889109
C	2.739513	0.197223	1.268950
C	2.263660	1.278928	0.470305
C	2.951760	0.218926	2.754756
H	2.780149	-0.765620	3.198583
H	3.976670	0.518643	2.999649
H	2.274481	0.923193	3.245043
C	1.900217	2.658029	0.939611
H	1.702015	2.675904	2.014098
H	2.716940	3.360327	0.739631
H	1.006345	3.026328	0.429268
C	1.774460	1.670740	-2.058020
H	0.858616	2.221080	-1.827029
H	2.546942	2.395723	-2.336752
H	1.571601	1.042753	-2.928530
C	2.776553	-1.355328	-2.170833
H	1.907489	-1.227730	-2.822858
H	3.669472	-1.081666	-2.742955
H	2.851778	-2.417187	-1.924388
C	3.519599	-2.252466	0.824199
H	4.613581	-2.259772	0.765694
H	3.241344	-2.493517	1.853404
H	3.147088	-3.056903	0.184754
Al	0.790225	-0.409828	0.251874
C	-1.355778	-0.259325	-0.327119
C	-2.216300	-1.347985	-0.094324
C	-3.510985	-1.147772	0.340244
C	-3.232861	1.200212	0.170165
C	-1.935853	1.020579	-0.267309
F	-0.430922	-0.436925	-1.506092
F	-1.134494	2.092292	-0.449332
F	-3.692804	2.450042	0.294661
F	-4.252211	-2.220807	0.636150
F	-1.695230	-2.584541	-0.110411
C	-4.063676	0.123481	0.451989
H	-5.090897	0.267019	0.757711

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0 1

Al	-0.919566	1.089889	-0.042165
F	0.000351	-0.000344	-1.220421
C	-2.655798	0.128678	0.012657
C	-3.196296	-0.357728	1.191536
C	-4.401824	-1.051044	1.237692
C	-5.135074	-1.256315	0.079046
C	-4.631769	-0.753611	-1.112454
C	-3.418025	-0.080321	-1.124871
C	-1.431171	3.000030	1.011076
C	-1.998817	3.076054	-0.293036
C	-0.947152	2.950908	-1.241177
C	0.291655	2.861184	-0.519238
C	-0.010889	2.894911	0.873622
C	-2.181415	3.052762	2.311319
H	-3.140222	2.529001	2.245238
H	-2.388561	4.087866	2.605573
H	-1.608005	2.584304	3.115932
C	-3.462169	3.188885	-0.599718
H	-4.065808	2.683416	0.160534
H	-3.703007	2.738718	-1.566854
H	-3.773388	4.238856	-0.630279
C	-1.058443	2.981496	-2.738763
H	-2.067931	2.729283	-3.070480
H	-0.370855	2.265557	-3.199729
H	-0.812321	3.975997	-3.128032
C	1.644769	2.848993	-1.169514
H	2.440644	2.671770	-0.441653
H	1.838147	3.814185	-1.651439
H	1.717781	2.074090	-1.939793
C	0.960476	2.846106	2.018595
H	0.883853	3.759482	2.617720
H	1.990561	2.766663	1.662941
H	0.777093	1.992242	2.676612
Al	0.920005	-1.090359	-0.041781
F	0.000247	0.000019	1.125547
C	2.656227	-0.129098	0.012855
C	3.418602	0.079746	-1.124598
C	4.631916	0.753813	-1.112250
C	5.134567	1.257577	0.079080
C	4.401116	1.052554	1.237642
C	3.196072	0.358385	1.191590
C	0.947659	-2.951693	-1.240332
C	1.998896	-3.076704	-0.291690
C	1.430672	-3.000207	1.012150
C	0.010450	-2.894950	0.874013
C	-0.291453	-2.861594	-0.518966
C	1.059499	-2.982727	-2.737867
H	2.069288	-2.731324	-3.069280
H	0.812809	-3.977150	-3.126978
H	0.372594	-2.266410	-3.199271
C	3.462361	-3.189790	-0.597731
H	3.703555	-2.740262	-1.565073
H	4.065743	-2.683820	0.162391
H	3.773571	-4.239786	-0.627461
C	2.180184	-3.052661	2.312825
H	3.139839	-2.530489	2.246605
H	1.607119	-2.582397	3.116635
H	2.385562	-4.087752	2.608368
C	-0.961367	-2.845674	2.018578
H	-1.991352	-2.767121	1.662431
H	-0.884477	-3.758494	2.618517
H	-0.778704	-1.991149	2.675933
C	-1.644272	-2.849215	-1.169854
H	-1.837462	-3.814294	-1.652077
H	-2.440460	-2.672131	-0.442298
H	-1.716936	-2.074138	-1.939988
F	2.961575	-0.365891	-2.315106
F	5.308500	0.924558	-2.251959
F	-2.543196	-0.169057	2.355147
F	-4.846901	-1.519242	2.407866
F	-5.308171	-0.924571	-2.252239
F	-2.960457	0.364439	-2.315505
F	2.542731	0.170092	2.355115
F	4.845475	1.521883	2.407643
H	-6.077601	-1.789415	0.104238
H	6.076728	1.791327	0.104215

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Al	1.002578	-1.403665	-0.174453
F	1.207952	-0.125100	1.155036
C	-0.966766	-1.588994	-0.071312
C	-1.839395	-1.301174	-1.107742
C	-3.219055	-1.399913	-0.973642
C	-3.779095	-1.819016	0.223796
C	-2.928683	-2.117924	1.277245
C	-1.554497	-2.000274	1.114019
C	1.508628	-3.198123	-1.458438
C	1.205812	-3.692388	-0.158599
C	2.098814	-3.087055	0.764299
C	3.004369	-2.254855	0.022307
C	2.640233	-2.332920	-1.356040
C	0.764455	-3.531559	-2.719918
H	-0.319237	-3.511338	-2.562437
H	1.027485	-4.530946	-3.084125
H	0.991456	-2.813311	-3.512386
C	0.088758	-4.639011	0.162549
H	-0.777313	-4.458585	-0.482264

H	-0.241432	-4.531603	1.198776
H	0.406159	-5.677001	0.013531
C	2.178536	-3.304210	2.248174
H	1.258352	-3.743565	2.637276
H	2.341136	-2.359049	2.776673
H	3.009195	-3.973940	2.499298
C	4.169532	-1.535574	0.639221
H	4.844167	-1.141564	-0.124017
H	4.744198	-2.220847	1.271376
H	3.848969	-0.698632	1.269868
C	3.310628	-1.651085	-2.516074
H	3.488009	-2.366069	-3.325164
H	4.280241	-1.240325	-2.222902
H	2.707345	-0.830878	-2.919506
Al	0.965560	1.427422	0.174496
F	1.203660	0.154817	-1.155216
C	-1.007498	1.562616	0.071044
C	-1.605094	1.957450	-1.115059
C	-2.981686	2.040602	-1.278634
C	-3.824583	1.722580	-0.224697
C	-3.254534	1.319546	0.973488
C	-1.872807	1.254969	1.107816
C	2.019917	3.136902	-0.764246
C	1.108952	3.722146	0.154021
C	1.419600	3.239237	1.456177
C	2.572807	2.402511	1.360137
C	2.943726	2.329913	-0.016822
C	2.098736	3.351830	-2.248501
H	1.166373	3.759846	-2.642848
H	2.908357	4.047141	-2.498756
H	2.293880	2.410594	-2.772976
C	-0.030345	4.639652	-0.173336
H	-0.353449	4.522387	-1.210714
H	-0.894144	4.438677	0.468443
H	0.260196	5.685565	-0.024838
C	0.661926	3.556029	2.713877
H	-0.420242	3.504524	2.552828
H	0.906409	2.847207	3.509623
H	0.895274	4.563715	3.075406
C	3.255792	1.740252	2.524187
H	4.235269	1.350784	2.234828
H	3.414678	2.461930	3.331181
H	2.670470	0.907836	2.928968
C	4.129071	1.638832	-0.627452
H	4.688494	2.336682	-1.259510
H	4.810665	1.264277	0.139367
H	3.832108	0.792194	-1.256682
F	-0.825575	2.278934	-2.170048
F	-3.487819	2.428357	-2.452127
F	-1.351602	-0.869700	-2.287413
F	-4.006970	-1.057626	-1.998759
F	-3.425101	-2.520207	2.450016
F	-0.767357	-2.303633	2.168763
F	-4.033771	0.959999	1.999286
F	-1.374754	0.837811	2.288363
H	-4.853748	-1.886996	0.341534
H	-4.900587	1.763632	-0.342586

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C	2.435397	0.842473	0.918303
C	1.572311	-0.258538	1.187506
C	1.762246	-1.225427	0.159866
C	3.161695	0.554964	-0.271445
C	2.741887	-0.720630	-0.743062
C	4.210397	1.427780	-0.898027
H	4.014926	2.487152	-0.709566
H	5.203598	1.198291	-0.495282
H	4.253671	1.288280	-1.981870
C	3.270386	-1.439299	-1.950512
H	3.596415	-0.739472	-2.725078
H	4.130248	-2.067055	-1.689146
H	2.510085	-2.090348	-2.391800
C	1.094140	-2.565944	0.049305
H	0.805719	-2.786061	-0.984156
H	1.767778	-3.365456	0.378806
H	0.192823	-2.619784	0.664504
C	0.662527	-0.370927	2.377093
H	-0.108101	-1.131655	2.231586
H	1.229571	-0.643937	3.274612
H	0.151179	0.573615	2.586278
C	2.581809	2.067052	1.774422
H	1.647779	2.305985	2.290843
H	3.353538	1.921106	2.539161
H	2.865438	2.941530	1.182096
Al	0.912175	0.702459	-0.822777
C	-2.274041	-1.284330	0.437524
C	-2.477331	0.028580	0.848175
C	-2.722399	1.009278	-0.101340
C	-2.763317	0.664436	-1.447833
C	-2.557592	-0.641807	-1.854864
C	-2.304715	-1.627684	-0.902418
F	-2.038420	-2.209722	1.377694
F	-2.978523	1.632923	-2.337274
F	-2.893725	2.270126	0.278965
F	-2.435657	0.347296	2.139097
H	-2.135644	-2.660448	-1.183629
H	-2.580761	-0.869192	-2.913747

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C	1.959737	-1.229462	0.608852
C	2.932062	-0.452262	-0.099271
C	2.720500	0.921997	0.229122
C	1.199722	-0.335420	1.428067
C	1.654809	0.984318	1.189222
C	0.065981	-0.711717	2.334491
H	-0.425346	-1.628861	1.999158
H	0.419528	-0.875362	3.358568
H	-0.692493	0.077198	2.364589
C	1.074282	2.220826	1.812164
H	-0.020387	2.213468	1.765396
H	1.359850	2.297872	2.866671
H	1.423994	3.126297	1.309386
C	3.539367	2.064301	-0.303512
H	3.018352	3.019174	-0.197474
H	4.491129	2.144906	0.232878
H	3.766239	1.925943	-1.364762
C	3.969284	-0.957934	-1.057599
H	4.004590	-0.345193	-1.962312
H	4.962652	-0.943105	-0.595588
H	3.759188	-1.984897	-1.364611
C	1.822045	-2.726189	0.580754
H	2.164860	-3.141803	-0.370289
H	2.414886	-3.185467	1.378824
H	0.781366	-3.029879	0.716045
Al	0.954455	0.143835	-0.789949
C	-0.981314	0.459242	-0.615844
C	-1.766497	-0.659754	-0.390685
C	-3.135710	-0.611898	-0.175339
C	-3.758436	0.629701	-0.192327
C	-3.029202	1.787011	-0.415029
C	-1.653912	1.690589	-0.624442
F	1.335843	0.108955	-2.418819
F	-5.077127	0.678860	0.014592
F	-3.841103	-1.721756	0.042187
F	-1.180433	-1.879980	-0.359640
H	-1.096953	2.607209	-0.800309
H	-3.550285	2.737832	-0.423446

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C	3.075798	-0.815597	0.220438
C	2.720340	-0.145741	-0.992460
C	2.171558	1.122236	-0.647975
C	2.747671	0.045899	1.309071
C	2.179774	1.236755	0.774762
C	2.946012	-0.263064	2.764308
H	2.932601	-1.340941	2.947565
H	3.907350	0.121518	3.122903
H	2.160517	0.183365	3.380801
C	1.689669	2.415762	1.566380
H	1.418713	2.124364	2.584274
H	2.462151	3.189442	1.637659
H	0.805037	2.870041	1.110348
C	1.693111	2.144320	-1.639319
H	1.252775	3.009322	-1.135421
H	2.524865	2.510305	-2.251044
H	0.941392	1.724185	-2.315975
C	2.905878	-0.643221	-2.396438
H	2.040990	-0.394021	-3.019203
H	3.791164	-0.189987	-2.856856
H	3.034827	-1.728103	-2.425800

C	3.729168	-2.162969	0.327069
H	3.472733	-2.800719	-0.522927
H	4.820103	-2.064633	0.351941
H	3.422692	-2.687023	1.236359
Al	0.824656	-0.496073	0.135706
C	-1.296680	-0.013197	-0.420222
C	-2.231208	-1.026952	-0.158744
C	-3.526236	-0.714064	0.201763
C	-3.952895	0.612887	0.183775
C	-3.068917	1.623096	-0.154412
C	-1.755804	1.313354	-0.492990
F	-0.286787	-0.365041	-1.558884
F	-5.225946	0.878434	0.499821
F	-4.373894	-1.683446	0.545118
F	-1.822731	-2.297114	-0.080304
H	-1.062214	2.102461	-0.761478
H	-3.425421	2.646864	-0.169130
H	-2.424534	2.673767	-0.164091
H	-1.937911	3.769060	-1.465612
H	-1.854463	2.018223	-1.702304
C	-0.723751	2.846266	2.129568
H	-0.767736	3.833947	2.601767
H	-1.743542	2.539638	1.886689
H	-0.333486	2.140486	2.869588
H	2.524420	-0.089977	-2.487624
H	4.761384	-1.151742	-2.755306
H	-4.761388	1.151722	2.755314
H	-2.524430	0.089943	2.487630
F	3.102846	0.199298	1.975103
F	5.522103	-0.921592	1.667184
F	6.390349	-1.639701	-0.784411
F	-3.102803	-0.199201	-1.975111
F	-5.522062	0.921681	-1.667188
F	-6.390327	1.639742	0.784413

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Al	-0.943845	-1.071520	0.076271
F	0.123487	-0.011377	1.172894
C	-2.656202	-0.128890	0.347140
C	-3.502556	0.113441	-0.722646
C	-4.753387	0.702580	-0.599881
C	-5.187293	1.070996	0.667733
C	-4.390721	0.852730	1.780993
C	-3.142630	0.253446	1.607005
C	-1.565338	-3.017718	-0.905717
C	-2.005856	-3.089431	0.444356
C	-0.871823	-2.943117	1.288093
C	0.293300	-2.846841	0.454933
C	-0.139810	-2.888226	-0.902735
C	-2.426671	-3.144684	-2.129292
H	-3.439002	-2.773659	-1.948803
H	-2.504920	-4.192507	-2.441414
H	-2.016408	-2.576559	-2.968764
C	-3.434222	-3.215030	0.883189
H	-4.103074	-2.638682	0.236034
H	-3.574814	-2.847389	1.903194
H	-3.759527	-4.260897	0.855071
C	-0.841122	-2.946447	2.790360
H	-1.818454	-2.697704	3.213062
H	-0.115744	-2.221375	3.173157
H	-0.555884	-3.931688	3.176648
C	1.702664	-2.819381	0.971688
H	2.424519	-2.673815	0.164081
H	1.937893	-3.769111	1.465599
H	1.854458	-2.018276	1.702301
C	0.723733	-2.846287	-2.129572
H	0.767703	-3.833964	-2.601780
H	1.743529	-2.539674	-1.886694
H	0.333474	-2.140495	-2.869584
Al	0.943840	1.071498	-0.076265
F	-0.123484	0.011347	-1.172887
C	2.656202	0.128883	-0.347137
C	3.502567	-0.113421	0.722647
C	4.753407	-0.702540	0.599881
C	5.187306	-1.070976	-0.667729
C	4.390722	-0.852739	-1.780987
C	3.142628	-0.253459	-1.607001
C	1.565322	3.017697	0.905716
C	2.005839	3.089417	-0.444356
C	0.871809	2.943093	-1.288094
C	-0.293315	2.846808	-0.454936
C	0.139794	2.888204	0.902733
C	2.426655	3.144662	2.129291
H	3.438989	2.773648	1.948799
H	2.504896	4.192484	2.441420
H	2.016397	2.576529	2.968761
C	3.434205	3.215027	-0.883189
H	4.103061	2.638686	-0.236031
H	3.574800	2.847380	-1.903192
H	3.759501	4.260896	-0.855077
C	0.841112	2.946422	-2.790361
H	1.818445	2.697679	-3.213060
H	0.115735	2.221348	-3.173160
H	0.555874	3.931662	-3.176650
C	-1.702677	2.819334	-0.971695

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Al	1.014253	-1.428080	0.035386
F	1.263922	0.041417	1.166304
C	-0.937368	-1.564497	0.251033
C	-1.792754	-1.511493	-0.836326
C	-3.176071	-1.526470	-0.721488
C	-3.736616	-1.616735	0.545802
C	-2.933142	-1.690989	1.672851
C	-1.548993	-1.660141	1.511359
C	1.516750	-3.431251	-0.935828
C	1.192838	-3.713756	0.418495
C	2.072404	-2.970703	1.247978
C	2.996330	-2.270506	0.399252
C	2.651643	-2.564723	-0.954523
C	0.791372	-3.964981	-2.137804
H	-0.294148	-3.917994	-2.002643
H	1.057636	-5.010479	-2.330053
H	1.032771	-3.385814	-3.033259
C	0.056616	-4.588018	0.855198
H	-0.832844	-4.414821	0.240850
H	-0.224295	-4.399329	1.894568
H	0.327357	-5.646133	0.766232
C	2.119594	-2.939907	2.749544
H	1.184642	-3.299210	3.187545
H	2.293857	-1.924372	3.120768
H	2.927955	-3.574070	3.131810
C	4.158381	-1.467313	0.909364
H	4.845414	-1.205369	0.101600
H	4.720935	-2.043974	1.651415
H	3.835736	-0.537438	1.390958
C	3.349154	-2.088784	-2.198214
H	3.538092	-2.930303	-2.871763
H	4.315020	-1.636290	-1.959364
H	2.758527	-1.347134	-2.746459
Al	1.017889	1.426273	-0.035491
F	1.263261	-0.043983	-1.166580
C	-0.933438	1.566923	-0.250763
C	-1.544689	1.663361	-1.511258
C	-2.928715	1.696371	-1.673039
C	-3.732519	1.623407	-0.546113
C	-3.172384	1.532380	0.721281
C	-1.789087	1.515344	0.836404
C	2.082604	2.964256	-1.247831
C	1.202407	3.711157	-0.422517
C	1.521723	3.430873	0.933359
C	2.654248	2.561535	0.957328
C	3.002275	2.263564	-0.394854
C	2.134476	2.930411	-2.749170
H	1.201504	3.290292	-3.190901
H	2.945074	3.562518	-3.130099
H	2.308275	1.913857	-3.117791
C	0.069529	4.587309	-0.864091
H	-0.207136	4.399238	-1.904714
H	-0.822848	4.415596	-0.253556
H	0.341688	5.644957	-0.773889
C	0.793579	3.968720	2.131793
H	-0.291636	3.921852	1.993995
H	1.032461	3.392330	3.029704
H	1.059842	5.014713	2.321307
C	3.346459	2.085494	2.203962
H	4.311241	1.628807	1.968733
H	3.536723	2.927592	2.876410
H	2.751511	1.347119	2.751928
C	4.164473	1.457397	-0.899862
H	4.731886	2.032705	-1.639275
H	4.847191	1.193458	-0.089117

H	3.841574	0.528500	-1.383111
F	-1.284636	-1.400799	-2.082105
F	-3.957361	-1.405160	-1.796593
F	-3.954056	1.412340	1.796239
F	-1.281404	1.403801	2.082287
F	-5.064025	1.612642	-0.648991
F	-5.068124	-1.604132	0.648509
H	-0.923900	1.687361	-2.404603
H	-3.399770	1.745594	-2.648284
H	-0.928438	-1.685181	2.404844
H	-3.404398	-1.739630	2.648022

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C	-3.112825	-0.796019	-0.591678
C	-2.327371	-1.137753	0.545553
C	-1.916569	0.069791	1.176875
C	-3.179168	0.625692	-0.667884
C	-2.437055	1.160023	0.425191
C	-3.933242	1.417685	-1.697261
H	-3.994126	0.882169	-2.648821
H	-4.958330	1.618559	-1.365302
H	-3.454972	2.381410	-1.893249
C	-2.246714	2.614465	0.748782
H	-2.403658	3.241837	-0.132659
H	-2.952818	2.943869	1.519515
H	-1.234990	2.810736	1.116315
C	-1.143253	0.156795	2.461011
H	-0.266841	-0.496250	2.454867
H	-0.794896	1.175336	2.646423
H	-1.775696	-0.138784	3.306182
C	-2.006185	-2.518604	1.039216
H	-0.993888	-2.564008	1.451793
H	-2.701926	-2.825250	1.829047
H	-2.070638	-3.257989	0.236377
C	-3.782056	-1.761272	-1.527278
H	-3.229162	-2.702382	-1.594132
H	-4.797319	-1.997266	-1.188381
H	-3.858868	-1.352827	-2.538914
Al	-0.971539	0.003015	-0.948992
C	2.328485	-0.709040	0.388731
C	3.299694	-1.334126	-0.385239
C	4.201229	-0.590476	-1.126200
C	4.131388	0.801369	-1.099437
C	3.161337	1.422036	-0.332320
C	2.260223	0.674473	0.417339
F	1.454695	-1.435528	1.086248
F	1.320619	1.280954	1.141290
F	3.062889	2.751886	-0.291279
F	3.335857	-2.667690	-0.394682
H	4.945678	-1.109244	-1.718136
H	4.818409	1.414075	-1.670644

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C	2.178656	-1.050842	0.498732
C	2.822728	0.064511	-0.127392
C	2.178511	1.255816	0.331042
C	1.193285	-0.536376	1.401773
C	1.182633	0.875176	1.293498
C	0.274205	-1.360875	2.252777
H	0.058945	-2.325310	1.784907
H	0.716646	-1.554803	3.236144
H	-0.681406	-0.851587	2.410059
C	0.256799	1.800944	2.027380
H	-0.739673	1.360791	2.135957
H	0.636103	2.016531	3.032025
H	0.137039	2.750932	1.501748
C	2.545501	2.654477	-0.079195
H	2.840585	2.694429	-1.131507
H	1.708186	3.343825	0.056049
H	3.384486	3.028887	0.517353
C	3.934955	0.013431	-1.132341
H	3.783098	0.746490	-1.928547
H	4.898407	0.223207	-0.654738
H	4.001069	-0.969781	-1.603490
C	2.518793	-2.504294	0.317015
H	3.033072	-2.678139	-0.631325
H	3.174018	-2.854982	1.121442
H	1.618601	-3.125051	0.323064
Al	0.742629	0.034312	-0.754585
C	-1.188488	-0.262166	-0.526086
C	-1.739189	-1.530935	-0.407763
C	-3.081150	-1.786011	-0.177612
C	-3.944210	-0.697265	-0.054666
C	-3.440501	0.588068	-0.160490
C	-2.082532	0.783402	-0.393097
F	1.052871	0.170414	-2.390980
F	-1.628432	2.050014	-0.477577
F	-4.246056	1.649689	-0.039538
F	-0.894019	-2.587574	-0.510411
H	-3.437536	-2.806355	-0.098949
H	-5.005057	-0.830398	0.124530

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C	-2.906716	-0.656685	-0.281357
C	-2.427840	-0.285099	1.015126
C	-1.806894	0.992139	0.905157
C	-2.585865	0.401378	-1.186738
C	-1.899870	1.414717	-0.456411
C	-2.912217	0.427327	-2.651697
H	-2.929978	-0.581049	-3.074666
H	-3.895586	0.877320	-2.827654
H	-2.176814	1.006856	-3.216163
C	-1.370544	2.711373	-0.999650
H	-1.291952	2.682523	-2.089176
H	-2.033615	3.542591	-0.736399
H	-0.376902	2.930954	-0.599777
C	-1.177354	1.744748	2.042143
H	-0.415636	1.140702	2.544116
H	-0.694170	2.658262	1.689903
H	-1.934059	2.023461	2.783375
C	-2.553555	-1.066798	2.290203
H	-1.636414	-0.997595	2.883026
H	-3.377588	-0.682378	2.901708
H	-2.747199	-2.125053	2.097455
C	-3.668558	-1.905482	-0.619162
H	-3.396756	-2.732059	0.042509
H	-4.747010	-1.740043	-0.519317
H	-3.476444	-2.227289	-1.646181
Al	-0.661720	-0.479543	-0.315858
C	1.514649	-0.614329	0.164270
C	2.278268	-1.734039	-0.217723
C	3.582076	-1.628113	-0.645950
C	4.231393	-0.389493	-0.620766
C	3.513282	0.717838	-0.196807
C	2.205919	0.602798	0.241730
F	0.584577	-0.856165	1.345629
F	1.511656	1.710023	0.574706
F	4.078996	1.931913	-0.180472
F	1.633938	-2.912389	-0.285368
H	4.090045	-2.524351	-0.984157
H	5.262904	-0.272886	-0.927117

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Al	1.000632	-0.974349	0.033009
F	-0.138382	-0.098192	-1.119511
C	2.633563	0.095467	-0.303562
C	3.476983	0.487497	0.720326
C	4.643154	1.215906	0.516444
C	5.010824	1.580350	-0.768244
C	4.208171	1.196042	-1.841537
C	3.060164	0.462569	-1.574283
C	1.318275	-2.693088	1.398215
C	2.273495	-2.840613	0.356294
C	1.570493	-2.948199	-0.877054
C	0.168171	-2.935524	-0.593959
C	0.008616	-2.775067	0.813646
C	1.585667	-2.552481	2.869541
H	2.592549	-2.174258	3.059409
H	1.484134	-3.517322	3.379562
H	0.879402	-1.856531	3.332869
C	3.764975	-2.807945	0.506771
H	4.064361	-2.248489	1.397674
H	4.239761	-2.332143	-0.357147
H	4.169805	-3.822205	0.595202
C	2.185608	-3.081288	-2.240736

H	3.098278	-2.483805	-2.329663
H	1.495932	-2.740159	-3.017718
H	2.446978	-4.123477	-2.456754
C	-0.916116	-3.083189	-1.623464
H	-1.907222	-3.059378	-1.163939
H	-0.813498	-4.040646	-2.144958
H	-0.885001	-2.285152	-2.370392
C	-1.266231	-2.786894	1.606425
H	-1.325074	-3.699846	2.210201
H	-2.146503	-2.753425	0.959600
H	-1.324320	-1.932734	2.288979
Al	-1.033648	1.026810	0.036549
F	0.103094	0.148020	1.201696
C	-2.674297	-0.060058	0.261033
C	-3.291129	-0.715370	-0.789305
C	-4.427339	-1.506125	-0.629199
C	-5.009266	-1.639167	0.619416
C	-4.444930	-0.973357	1.708199
C	-3.307344	-0.215178	1.488374
C	-1.787067	2.774618	-1.147015
C	-2.249049	2.946940	0.188723
C	-1.115900	3.001186	1.045032
C	0.061873	2.927418	0.226458
C	-0.356313	2.790161	-1.129244
C	-2.645457	2.626435	-2.370762
H	-3.532616	2.017574	-2.169573
H	-2.987364	3.601734	-2.735371
H	-2.093742	2.140462	-3.180257
C	-3.686829	2.979856	0.612785
H	-4.303435	2.344381	-0.030601
H	-3.807739	2.624962	1.640075
H	-4.085824	3.998871	0.558894
C	-1.104050	3.182434	2.535953
H	-2.060336	2.899303	2.980829
H	-0.328339	2.566296	3.001374
H	-0.901998	4.226616	2.800870
C	1.460989	3.075708	0.750299
H	2.205058	2.901307	-0.030925
H	1.611212	4.089118	1.139865
H	1.665600	2.373801	1.565578
C	0.520729	2.688729	-2.344676
H	0.306353	3.511243	-3.035221
H	1.577546	2.745976	-2.073213
H	0.373157	1.747181	-2.880952
H	-4.867922	-1.047608	2.703234
H	4.463904	1.450401	-2.863727
F	-2.787674	-0.605191	-2.034182
F	-4.942763	-2.131883	-1.694986
F	3.156097	0.170687	1.993485
F	5.396955	1.562168	1.567264
H	5.920660	2.151944	-0.912694
H	-5.895349	-2.255029	0.723834
F	-2.750579	0.408788	2.557163
F	2.305274	0.078092	-2.630325

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Al	1.433921	0.796400	-0.039722
F	0.042365	1.040905	1.163531
C	1.567322	-1.172063	0.059492
C	1.354527	-2.033463	-1.001684
C	1.413972	-3.417928	-0.873755
C	1.705709	-3.990605	0.352222
C	1.931314	-3.167087	1.454291
C	1.855014	-1.796680	1.267282
C	3.362782	1.266039	-1.145562
C	3.721731	0.952681	0.194778
C	3.047130	1.856754	1.056530
C	2.309235	2.778936	0.239524
C	2.513197	2.413036	-1.125590
C	3.799647	0.511553	-2.368572
H	3.728753	-0.570909	-2.216410
H	4.838955	0.742031	-2.628406
H	3.173621	0.760769	-3.229670
C	4.608896	-0.184738	0.601999
H	4.459761	-1.051891	-0.049348
H	4.405407	-0.502879	1.627329
H	5.663807	0.104684	0.538462
C	3.119491	1.929453	2.554755
H	3.475789	0.990568	2.982487
H	2.134062	2.133928	2.986209
H	3.796614	2.729963	2.874803
C	1.557372	3.958843	0.785564
H	1.256966	4.643138	-0.010980
H	2.187898	4.517399	1.485548
H	0.654216	3.655931	1.327272
C	1.960013	3.096682	-2.344917
H	2.752203	3.255551	-3.082881
H	1.546228	4.076354	-2.092095
H	1.167556	2.511886	-2.823917
Al	-1.416745	0.824451	0.040374
F	-0.020546	1.041361	-1.163031
C	-1.590217	-1.140760	-0.059232
C	-1.888484	-1.759132	-1.267653
C	-1.992007	-3.127684	-1.455067
C	-1.784496	-3.955758	-0.352856
C	-1.482784	-3.389369	0.873651
C	-1.395761	-2.006409	1.002011
C	-3.007400	1.918030	-1.056741
C	-3.701785	1.025703	-0.198535
C	-3.339952	1.328942	1.143256
C	-2.467028	2.458256	1.127911
C	-2.252785	2.823286	-0.236030
C	-3.074868	1.995129	-2.554964
H	-3.447291	1.063741	-2.985401
H	-3.736481	2.808513	-2.874997
H	-2.084861	2.182421	-2.983721
C	-4.610685	-0.092796	-0.610080
H	-4.410779	-0.413600	-1.635270
H	-4.481172	-0.963695	0.040477
H	-5.659689	0.217923	-0.549116
C	-3.794498	0.580333	2.363407
H	-3.741250	-0.503010	2.210152
H	-3.167982	0.817959	3.227402
H	-4.830842	0.827974	2.619213
C	-1.902185	3.127599	2.349846
H	-1.464208	4.097292	2.099353
H	-2.692980	3.304787	3.085146
H	-1.125540	2.523850	2.831186
C	-1.476449	3.989358	-0.777478
H	-2.094256	4.562154	-1.477315
H	-1.164161	4.665511	0.021459
H	-0.578377	3.669975	-1.318088
F	-2.091697	-0.956484	-2.342865
F	1.044669	-1.531037	-2.212451
F	1.157194	-4.186444	-1.941032
F	2.076135	-0.998691	2.342433
F	-1.243192	-4.163244	1.941045
F	-1.077519	-1.510365	2.213246
H	-2.212099	-3.529477	-2.436999
H	-1.832151	-5.035867	-0.435238
H	1.731796	-5.071464	0.434384
H	2.144727	-3.573451	2.435813

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C	2.486300	1.124429	-0.023618
C	3.045726	-0.020719	0.609158
C	2.467549	-1.175352	0.011952
C	1.576542	0.678239	-1.024029
C	1.559841	-0.744226	-0.999066
C	0.817447	1.584387	-1.953422
H	0.067388	2.191840	-1.434888
H	1.503170	2.271199	-2.461388
H	0.301786	1.009758	-2.727057
C	0.767129	-1.658232	-1.889122
H	-0.009678	-1.115920	-2.433565
H	1.415239	-2.144214	-2.627442
H	0.264333	-2.447035	-1.320606
C	2.786089	-2.604826	0.342233
H	1.927762	-3.256398	0.153577
H	3.619694	-2.973273	-0.267045
H	3.067685	-2.723641	1.392404
C	4.082472	-0.012004	1.694903
H	3.984608	-0.882439	2.349883
H	5.093828	-0.028281	1.272776
H	4.000334	0.881983	2.319683
C	2.823179	2.560435	0.256839
H	3.120778	2.709687	1.298581
H	3.651816	2.901284	-0.375264
H	1.967142	3.212710	0.059690
Al	0.765571	0.000937	1.056174
C	-3.056415	-0.195563	1.435244
C	-2.881788	1.114847	1.015509

C	-2.523257	1.307253	-0.309490
C	-2.347271	0.263405	-1.206249
C	-2.538016	-1.021747	-0.719353
C	-2.890765	-1.287118	0.595166
F	-3.391411	-0.417228	2.707999
H	-3.001961	1.947272	1.696477
H	-2.082399	0.445703	-2.239842
H	-3.027244	-2.299862	0.951490
F	-2.375329	-2.051350	-1.558488
F	-2.329401	2.558379	-0.744808

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C	1.605624	-0.928692	1.152452
C	2.650592	-0.785923	0.180331
C	2.747623	0.597171	-0.153557
C	1.089097	0.364838	1.439296
C	1.760914	1.307445	0.610854
C	-0.036112	0.635586	2.392935
H	-0.874847	-0.049125	2.224908
H	0.296156	0.513613	3.429887
H	-0.421562	1.651998	2.282644
C	1.546656	2.795829	0.588763
H	0.548516	3.060750	0.946684
H	2.273563	3.304133	1.231301
H	1.656495	3.206490	-0.419344
C	3.725661	1.176166	-1.134201
H	3.462980	2.203204	-1.399772
H	4.736402	1.190736	-0.711533
H	3.753169	0.588979	-2.056817
C	3.507818	-1.866839	-0.412475
H	3.565962	-1.769221	-1.500631
H	4.526652	-1.815793	-0.013296
H	3.112997	-2.860461	-0.187246
C	1.128498	-2.201522	1.792651
H	1.421839	-3.080803	1.213156
H	1.546139	-2.314089	2.799060
H	0.037398	-2.211033	1.886493
Al	0.807805	-0.153660	-0.791356
C	-1.145758	-0.084864	-0.602996
C	-1.897454	-1.263730	-0.480976
C	-3.265010	-1.196579	-0.249590
C	-3.944329	0.005488	-0.130235
C	-3.189338	1.161599	-0.256410
C	-1.820741	1.139573	-0.481156
F	1.203404	-0.523633	-2.376756
F	-3.813922	2.343860	-0.147139
F	-3.962867	-2.335754	-0.130960
H	-1.305661	2.093924	-0.558061
H	-1.447995	-2.249360	-0.569552
H	-5.011649	0.040111	0.049343

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C	3.013017	-0.626255	0.399751
C	2.596217	-0.326967	-0.937530
C	1.841888	0.882804	-0.902959
C	2.497320	0.386918	1.253262
C	1.764720	1.312981	0.454839
C	2.663455	0.477531	2.741736
H	2.812157	-0.508127	3.191443
H	3.528970	1.095894	3.006103
H	1.782246	0.925848	3.210793
C	1.063662	2.531393	0.988472
H	0.306199	2.272335	1.736299
H	1.778979	3.210462	1.464464
H	0.561245	3.086856	0.192945
C	1.258616	1.548512	-2.117496
H	0.771063	2.492785	-1.861692
H	2.045214	1.772777	-2.845630
H	0.517487	0.910369	-2.609953
C	2.937753	-1.086895	-2.186779
H	2.093710	-1.099564	-2.883469
H	3.789166	-0.628666	-2.703192
H	3.203366	-2.124285	-1.966872
C	3.868264	-1.786762	0.816824
H	3.715022	-2.652471	0.166497
H	4.930762	-1.522976	0.772766
H	3.646602	-2.098985	1.841008
Al	0.738107	-0.722486	0.227500
C	-1.456908	-0.561026	-0.238370
C	-2.379082	-1.565878	0.108217
C	-3.673991	-1.182524	0.395257
C	-4.131155	0.129029	0.314797
C	-3.201483	1.072116	-0.098360
C	-1.890400	0.766196	-0.415875
F	-0.446198	-0.988894	-1.367502
F	-3.595354	2.349101	-0.208306
F	-4.541971	-2.128329	0.780699
H	-1.219944	1.552175	-0.742451
H	-2.086816	-2.601672	0.216275
H	-5.150458	0.395612	0.558424

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Al	0.942956	-1.079348	-0.073294
F	0.018242	0.116143	-1.167868
C	2.659378	-0.112235	-0.025242
C	3.505176	-0.103488	1.095298
C	4.695911	0.607160	1.068013
C	5.111184	1.328479	-0.043088
C	4.276100	1.297473	-1.148981
C	3.077689	0.596062	-1.161251
C	1.485529	-3.122038	0.773704
C	2.063209	-3.049997	-0.522703
C	1.017932	-2.818371	-1.457359
C	-0.228882	-2.813675	-0.743814
C	0.066046	-3.000680	0.638309
C	2.198537	-3.362529	2.074275
H	3.257708	-3.100115	2.007155
H	2.138289	-4.417810	2.365091
H	1.758961	-2.776816	2.888851
C	3.526174	-3.110916	-0.847116
H	4.138335	-2.843914	0.018384
H	3.786844	-2.415178	-1.650525
H	3.813342	-4.118531	-1.167586
C	1.158304	-2.661748	-2.944982
H	2.153176	-2.296333	-3.215591
H	0.423022	-1.954028	-3.340128
H	1.005664	-3.617219	-3.459809
C	-1.579713	-2.750530	-1.395971
H	-2.379959	-2.611680	-0.664942
H	-1.774379	-3.680150	-1.943039
H	-1.645093	-1.923552	-2.109179
C	-0.906710	-3.132651	1.774677
H	-0.827633	-4.129245	2.223062
H	-1.936880	-2.994480	1.441075
H	-0.713284	-2.399236	2.564882
Al	-0.940496	1.075619	0.092491
F	-0.017274	-0.120314	1.185803
C	-2.657410	0.112302	0.007300
C	-3.462482	0.091002	-1.142996
C	-4.657994	-0.612222	-1.147894
C	-5.115818	-1.316385	-0.042527
C	-4.319674	-1.275164	1.091368
C	-3.119336	-0.578230	1.136979
C	-1.505187	3.128714	-0.716212
C	-2.056302	3.037351	0.590669
C	-0.991472	2.797312	1.500662
C	0.240173	2.803992	0.760674
C	-0.083684	3.008783	-0.612948
C	-2.255966	3.382886	-1.992250
H	-3.302190	3.075527	-1.908813
H	-2.244935	4.448768	-2.248556
H	-1.812782	2.842232	-2.835390
C	-3.516045	3.093825	0.929698
H	-4.126710	2.649064	0.138288
H	-3.733843	2.545642	1.850423
H	-3.844305	4.129732	1.069752
C	-1.089503	2.623002	2.989851
H	-2.085130	2.284484	3.289690
H	-0.364106	1.887071	3.350332
H	-0.889259	3.565644	3.511862
C	1.603169	2.741619	1.387314
H	2.391191	2.616336	0.640861
H	1.801815	3.666224	1.941545
H	1.686576	1.907282	2.090042
C	0.866214	3.157154	-1.766776

H	0.775295	4.158720	-2.201457
H	1.903172	3.018351	-1.455215
H	0.659609	2.432823	-2.562052
H	-2.548649	-0.606384	2.061993
H	-6.048398	-1.866474	-0.064902
H	6.041271	1.883218	-0.046139
H	2.473982	0.634351	-2.064534
F	-5.405986	-0.627150	-2.261980
F	-4.721317	-1.953049	2.178757
F	4.635931	1.991592	-2.240931
F	5.482741	0.611135	2.155195
H	-3.168941	0.597806	-2.059216
H	3.247921	-0.626421	2.013360

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Al	0.818572	-1.446575	-0.123597
F	1.073527	-0.109797	1.168396
C	-1.138477	-1.598859	-0.019730
C	-1.991134	-1.281459	-1.085648
C	-3.367542	-1.330881	-0.913397
C	-3.960363	-1.711876	0.280878
C	-3.105927	-2.037940	1.322580
C	-1.725900	-1.989939	1.194178
C	1.326260	-3.351672	-1.319333
C	0.987474	-3.784531	-0.010363
C	1.852998	-3.136623	0.907859
C	2.784629	-2.343003	0.153500
C	2.456175	-2.485410	-1.229758
C	0.601326	-3.746222	-2.574028
H	-0.482711	-3.634040	-2.457296
H	0.798086	-4.792377	-2.834323
H	0.910103	-3.127734	-3.421515
C	-0.138672	-4.723315	0.300134
H	-1.049452	-4.443819	-0.239568
H	-0.379894	-4.732143	1.365979
H	0.126537	-5.745875	0.008039
C	1.893610	-3.285120	2.402719
H	0.959742	-3.700276	2.790821
H	2.059810	-2.320390	2.893770
H	2.705060	-3.955165	2.710034
C	3.952324	-1.619210	0.760552
H	4.664007	-1.303156	-0.005587
H	4.483628	-2.276353	1.457323
H	3.643127	-0.729034	1.318814
C	3.176192	-1.880622	-2.403271
H	3.321943	-2.631927	-3.185174
H	4.164714	-1.516398	-2.111444
H	2.628127	-1.040824	-2.843813
Al	0.882470	1.410792	0.123424
F	1.077705	0.063928	-1.168162
C	-1.066358	1.647189	0.020102
C	-1.636630	2.064322	-1.193463
C	-3.013305	2.170480	-1.321830
C	-3.881027	1.878885	-0.280722
C	-3.305029	1.471646	0.912988
C	-1.931822	1.364545	1.085329
C	1.990703	3.052965	-0.908162
C	1.153209	3.738949	0.008422
C	1.471340	3.293052	1.318198
C	2.562498	2.378309	1.230830
C	2.886069	2.220232	-0.151947
C	2.039416	3.198130	-2.403095
H	1.124120	3.651305	-2.792946
H	2.878473	3.833444	-2.710016
H	2.165900	2.226752	-2.892858
C	0.069617	4.725798	-0.304472
H	-0.170044	4.743716	-1.370548
H	-0.853001	4.487555	0.234890
H	0.379304	5.736140	-0.013660
C	0.762255	3.719143	2.571632
H	-0.325450	3.655042	2.452782
H	1.041645	3.087350	3.419505
H	1.004674	4.755474	2.832720
C	3.253627	1.743610	2.405960
H	4.225188	1.335022	2.115900
H	3.431994	2.488744	3.186999
H	2.667964	0.929844	2.846966
C	4.023071	1.447378	-0.756857
H	4.588105	2.083782	-1.446340
H	4.714877	1.094373	0.011277
H	3.677122	0.575702	-1.322657
F	-3.534173	2.563765	-2.494776
F	-4.165655	-0.975649	-1.932580
F	-3.642785	-2.407023	2.496095
F	-4.117344	1.148557	1.931636
H	-1.126982	-2.246068	2.066205
H	-5.036544	-1.729110	0.401439
H	-1.610284	-0.939325	-2.044469
H	-4.955428	1.941391	-0.402148
H	-1.027103	2.296497	-2.064836
H	-1.566009	1.005323	2.043788

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C	2.307336	-1.144347	0.388193
C	2.860901	-0.347680	-0.652253
C	2.450639	0.997806	-0.440086
C	1.560427	-0.289861	1.248831
C	1.649511	1.035243	0.736535
C	0.848004	-0.723812	2.497045
H	0.363638	-1.696644	2.364969
H	1.545462	-0.813644	3.337909
H	0.072957	-0.007795	2.782694
C	1.050954	2.274288	1.337146
H	0.243677	2.030078	2.032313
H	1.805170	2.847201	1.889017
H	0.632632	2.932347	0.568545
C	2.829905	2.184639	-1.277565
H	2.050007	2.951531	-1.259398
H	3.754455	2.645870	-0.911061
H	2.992938	1.904507	-2.322051
C	3.745892	-0.835780	-1.762497
H	3.627755	-0.229535	-2.665069
H	4.801853	-0.793200	-1.471690
H	3.518965	-1.871604	-2.030062
C	2.507981	-2.620140	0.577603
H	2.655522	-3.131460	-0.377746
H	3.387980	-2.821285	1.199623
H	1.645739	-3.081306	1.067828
Al	0.533794	-0.266183	-0.843789
C	-3.163642	0.061285	-1.004058
C	-3.023458	-0.864148	0.024286
C	-2.642105	-0.456428	1.290389
C	-2.398113	0.897098	1.523353
C	-2.531500	1.822900	0.492258
C	-2.918532	1.404286	-0.780532
F	-3.513574	-0.375668	-2.215597
H	-2.110286	1.224961	2.517317
H	-3.023887	2.097210	-1.607856
H	-2.538392	-1.203020	2.070437
H	-2.336120	2.874403	0.674596
F	-3.245824	-2.154369	-0.238064

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C	-1.586444	-1.149684	-0.640105
C	-2.477016	-0.305710	0.096501
C	-2.136705	1.052040	-0.194437
C	-0.750314	-0.308113	-1.441259
C	-1.080228	1.039750	-1.165800
C	0.343004	-0.763705	-2.360818
H	0.734605	-1.738455	-2.058847
H	-0.019340	-0.849750	-3.391396
H	1.180099	-0.058023	-2.356406
C	-0.386673	2.231521	-1.758772
H	0.702507	2.124342	-1.704952
H	-0.656227	2.355605	-2.813135
H	-0.657500	3.154324	-1.239019
C	-2.840544	2.255474	0.368175
H	-2.221207	3.153395	0.298919
H	-3.771693	2.452936	-0.174100
H	-3.094525	2.109865	1.422172
C	-3.548873	-0.744889	1.049015
H	-3.594976	-0.089181	1.922063
H	-4.530211	-0.733867	0.561514
H	-3.366649	-1.758553	1.413124
C	-1.583063	-2.652827	-0.648739
H	-1.995399	-3.057816	0.278961
H	-2.185163	-3.039249	-1.478041
H	-0.568599	-3.044298	-0.756666
Al	-0.447857	0.071983	0.795219
C	1.495707	0.290372	0.613426
C	2.208410	-0.871810	0.357569

C	3.573374	-0.938826	0.135182
C	4.291359	0.254332	0.173156
C	3.634989	1.456729	0.426669
C	2.256697	1.467836	0.643472
F	-0.830013	-0.069166	2.419203
F	1.497675	-2.035502	0.310907
H	1.766633	2.419032	0.841420
H	4.196994	2.384904	0.457913
H	5.363685	0.240926	0.005191
H	4.048065	-1.894845	-0.056953

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C	-2.612334	-0.701161	-0.248130
C	-2.148837	-0.280247	1.038480
C	-1.547635	1.001468	0.889168
C	-2.294912	0.324873	-1.184777
C	-1.626096	1.369254	-0.486746
C	-2.582442	0.295839	-2.657596
H	-2.719448	-0.728186	-3.015059
H	-3.495137	0.853878	-2.894965
H	-1.765057	0.737144	-3.235968
C	-1.107478	2.644350	-1.088610
H	-0.945879	2.535442	-2.164054
H	-1.816796	3.466485	-0.941502
H	-0.153621	2.943608	-0.643771
C	-0.956332	1.806333	2.011092
H	-0.516280	2.736556	1.640529
H	-1.725912	2.076287	2.742511
H	-0.176217	1.246823	2.538147
C	-2.288556	-1.011698	2.341933
H	-1.381132	-0.914485	2.946322
H	-3.124253	-0.611363	2.927422
H	-2.472171	-2.078167	2.188109
C	-3.345419	-1.976863	-0.546384
H	-3.073243	-2.767713	0.157693
H	-4.429013	-1.829428	-0.478073
H	-3.122959	-2.342306	-1.552566
Al	-0.333583	-0.517904	-0.249114
C	1.839912	-0.182935	0.197371
C	2.730168	-1.154362	-0.283617
C	4.011796	-0.830676	-0.670884
C	4.482352	0.472517	-0.482860
C	3.639034	1.429193	0.076484
C	2.338001	1.104878	0.448332
F	0.880839	-0.701673	1.334560
F	2.258663	-2.394706	-0.485273
H	1.684481	1.851730	0.887881
H	3.996290	2.441013	0.240438
H	5.498202	0.726617	-0.763116
H	4.631867	-1.608348	-1.104605

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Al	-1.243261	-0.706434	0.047444
F	0.061665	-0.004795	1.177753
C	-2.584263	0.726487	0.211550
C	-3.277494	1.190306	-0.897095
C	-4.286760	2.140014	-0.867228
C	-4.639708	2.675737	0.369684
C	-3.985843	2.250227	1.524189
C	-2.979245	1.286898	1.436016
C	-2.401372	-2.405491	-0.919993
C	-2.906476	-2.281724	0.402954
C	-1.825460	-2.461684	1.307105
C	-0.650135	-2.765962	0.541927
C	-1.008693	-2.724879	-0.837420
C	-3.198816	-2.302408	-2.188148
H	-4.050699	-1.627499	-2.071473
H	-3.585277	-3.284160	-2.485867
H	-2.591128	-1.918782	-3.012444
C	-4.320216	-1.931882	0.760463
H	-4.736582	-1.194376	0.066837
H	-4.384870	-1.501616	1.763489
H	-4.961138	-2.820330	0.733165
C	-1.868339	-2.407709	2.808029
H	-2.734790	-1.844209	3.165231
H	-0.969304	-1.931046	3.211898
H	-1.928425	-3.414027	3.238584
C	0.672328	-3.151993	1.138968
H	1.442285	-3.270720	0.372743
H	0.576975	-4.104961	1.672489
H	1.031259	-2.404306	1.853604
C	-0.116715	-3.001700	-2.012387
H	-0.349475	-3.978964	-2.450123
H	0.936056	-3.000699	-1.721300
H	-0.242787	-2.247503	-2.795583
Al	1.243266	0.706429	-0.047438
F	-0.061651	0.004774	-1.177749
C	2.584290	-0.726477	-0.211547
C	3.277508	-1.190319	0.897097
C	4.286777	-2.140023	0.867222
C	4.639771	-2.675689	-0.369702
C	3.985934	-2.250140	-1.524209
C	2.979306	-1.286844	-1.436022
C	2.401382	2.405519	0.919979
C	2.906463	2.281743	-0.402975
C	1.825428	2.461688	-1.307108
C	0.650110	2.765944	-0.541907
C	1.008693	2.724865	0.837433
C	3.198859	2.302487	2.188118
H	4.050773	1.627620	2.071433
H	3.585280	3.284261	2.485813
H	2.591209	1.918843	3.012433
C	4.320201	1.931917	-0.760505
H	4.736577	1.194392	-0.066904
H	4.384852	1.501684	-1.763544
H	4.961119	2.820367	-0.733184
C	1.868279	2.407715	-2.808032
H	2.734740	1.844243	-3.165253
H	0.969251	1.931023	-3.211883
H	1.928323	3.414035	-3.238589
C	-0.672373	3.151957	-1.138916
H	-1.442315	3.270658	-0.372673
H	-0.577051	4.104934	-1.672428
H	-1.031305	2.404271	-1.853553
C	0.116725	3.001662	2.012414
H	0.349453	3.978940	2.450136
H	-0.936052	3.000613	1.721345
H	0.242843	2.247478	2.795614
H	4.767108	-2.449093	1.789466
H	2.477725	-0.970058	-2.350091
H	4.259836	-2.666982	-2.488599
H	5.424087	-3.424073	-0.427503
H	-4.767134	2.449031	-1.789468
H	-5.424017	3.424129	0.427478
H	-4.259708	2.667115	2.488570
H	-2.477644	0.970141	2.350084
F	2.923561	-0.697657	2.114933
F	-2.923685	0.697480	-2.114907

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Al	-1.422070	-0.517857	0.004008
F	0.018184	-0.789024	1.168328
C	-1.566196	1.425384	0.239831
C	-1.579283	2.304897	-0.831857
C	-1.699749	3.681951	-0.723640
C	-1.824061	4.227475	0.551518
C	-1.818898	3.395918	1.669555
C	-1.689632	2.017416	1.506220
C	-3.415774	-1.013345	-1.008935
C	-3.725923	-0.690721	0.339349
C	-3.002652	-1.573462	1.182366
C	-2.286266	-2.496948	0.347609
C	-2.550864	-2.149126	-1.011349
C	-3.925477	-0.290215	-2.222395
H	-3.932706	0.793006	-2.065970
H	-4.947818	-0.599640	-2.468653
H	-3.294439	-0.488054	-3.093317
C	-4.602387	0.449740	0.760898
H	-4.399385	1.345034	0.164099
H	-4.441978	0.716951	1.808556
H	-5.660150	0.191470	0.636252
C	-2.998780	-1.619014	2.684229
H	-3.356626	-0.679758	3.114185
H	-1.990923	-1.800708	3.072660
H	-3.645828	-2.421478	3.057580
C	-1.494471	-3.660443	0.871984
H	-1.197324	-4.334674	0.065592

H	-2.093727	-4.237390	1.584713
H	-0.585522	-3.337184	1.391827
C	-2.047852	-2.842612	-2.246407
H	-2.877491	-3.050260	-2.929444
H	-1.578711	-3.798307	-1.998816
H	-1.311201	-2.239267	-2.787477
Al	1.421660	-0.518461	-0.004324
F	-0.018718	-0.788944	-1.168647
C	1.566921	1.424688	-0.240077
C	1.690482	2.016735	-1.506412
C	1.820469	3.395207	-1.669662
C	1.826210	4.226649	-0.551577
C	1.701761	3.681087	0.723582
C	1.580584	2.304115	0.831713
C	3.000631	-1.576769	-1.182200
C	3.725265	-0.692954	-0.341464
C	3.416406	-1.013119	1.007701
C	2.550809	-2.148316	1.013000
C	2.284584	-2.498388	-0.345082
C	2.995395	-1.625051	-2.683970
H	3.352558	-0.686478	-3.115988
H	3.642343	-2.428002	-3.056446
H	1.987236	-1.807741	-3.071131
C	4.601939	0.446224	-0.766036
H	4.439506	0.712581	-1.813605
H	4.401109	1.342299	-0.169682
H	5.659722	0.187044	-0.643468
C	3.927441	-0.288042	2.219428
H	3.935888	0.794835	2.060690
H	3.296498	-0.483275	3.091006
H	4.949511	-0.598149	2.465949
C	2.048264	-2.839112	2.249758
H	1.577454	-3.794528	2.004266
H	2.878378	-3.046836	2.932196
H	1.313062	-2.233862	2.790661
C	1.491964	-3.662605	-0.866570
H	2.090917	-4.241973	-1.577597
H	1.194007	-4.334435	-0.058490
H	0.583439	-3.339969	-1.387523
F	-1.456003	1.781454	-2.079704
F	1.457102	1.780588	2.079489
H	1.670930	1.384717	-2.393625
H	1.909098	3.821040	-2.664528
H	1.919633	5.302199	-0.668328
H	1.684414	4.295900	1.617067
H	-1.670529	1.385305	2.393373
H	-1.907411	3.821755	2.664430
H	-1.916898	5.303066	0.668361
H	-1.681970	4.296766	-1.617116

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C	2.217622	-1.150240	-0.025280
C	2.726625	-0.000176	-0.689166
C	2.217653	1.150202	-0.025800
C	1.400308	-0.711467	1.055382
C	1.400327	0.711935	1.055060
C	0.707752	-1.612080	2.036832
H	0.262629	-2.480329	1.540032
H	1.410048	-1.986496	2.790658
H	-0.095488	-1.088272	2.561109
C	0.707791	1.613006	2.036106
H	-0.095329	1.089389	2.560755
H	1.410137	1.987895	2.789651
H	0.262517	2.480946	1.538900
C	2.520710	2.579903	-0.369243
H	1.687985	3.238822	-0.106388
H	3.405949	2.936090	0.170573
H	2.714555	2.704118	-1.438397
C	3.656817	-0.000469	-1.867586
H	3.506795	0.881514	-2.496715
H	4.703889	-0.000717	-1.543321
H	3.506356	-0.882432	-2.496641
C	2.520665	-2.580098	-0.368080
H	2.714746	-2.704742	-1.437141
H	3.405764	-2.936119	0.172074
H	1.687846	-3.238870	-0.105152
Al	0.396402	-0.000194	-0.927391
C	-3.386726	-0.000289	-1.080668
C	-3.195895	-1.214951	-0.439600
C	-2.802125	-1.206403	0.895894
C	-2.609140	0.000487	1.566136
C	-2.802062	1.206984	0.895166
C	-3.195830	1.214748	-0.440333
F	-3.759434	-0.000665	-2.368035
H	-3.348932	-2.136387	-0.990063
H	-2.648038	-2.147648	1.414758
H	-2.319923	0.000797	2.612676
H	-2.647926	2.148533	1.413464
H	-3.348821	2.135859	-0.991351

4h_Int2

0 1

C	1.847232	0.250113	1.152408
C	2.399618	-0.386388	0.000202
C	1.847633	0.250486	-1.152011
C	1.030137	1.343321	0.706215
C	1.030385	1.343546	-0.705781
C	0.303410	2.275355	1.633628
H	-0.522633	1.777153	2.154502
H	0.986625	2.671032	2.392224
H	-0.117752	3.126109	1.091945
C	0.304020	2.275986	-1.633071
H	-0.117496	3.126398	-1.091129
H	0.987564	2.672150	-2.391115
H	-0.521710	1.777985	-2.154632
C	2.154039	-0.075599	-2.587418
H	1.315099	0.184036	-3.239629
H	3.030564	0.480678	-2.938541
H	2.362168	-1.140616	-2.721857
C	3.330207	-1.561596	0.000079
H	3.173568	-2.190604	-0.879325
H	4.374218	-1.229181	-0.000446
H	3.174340	-2.190181	0.879921
C	2.152946	-0.076354	2.587875
H	2.361804	-1.141264	2.722006
H	3.028807	0.480457	2.939812
H	1.313380	0.182360	3.239648
Al	0.240856	-0.706686	-0.000243
C	-1.689953	-0.395830	-0.000213
C	-2.508661	-1.539194	-0.000215
C	-3.898982	-1.442519	-0.000166
C	-4.509408	-0.191420	-0.000133
C	-3.723476	0.958520	-0.000155
C	-2.334676	0.850381	-0.000187
F	0.412941	-2.377441	-0.000635
H	-2.046369	-2.522707	-0.000258
H	-4.505856	-2.343620	-0.000156
H	-5.592714	-0.111515	-0.000096
H	-4.192817	1.938375	-0.000146
H	-1.745214	1.764000	-0.000204

4h_TS

0 1

C	-2.590759	-0.055193	-0.640268
C	-2.128815	-0.924040	0.399984
C	-1.319305	-0.155969	1.287053
C	-2.044707	1.233166	-0.404950
C	-1.248436	1.172213	0.775122
C	-2.225509	2.458644	-1.251330
H	-2.496093	2.200949	-2.278983
H	-3.017108	3.104107	-0.852920
H	-1.305634	3.050977	-1.290642
C	-0.500098	2.339911	1.356289
H	0.292506	2.693815	0.687019
H	-1.178611	3.180165	1.538043
H	-0.033155	2.081935	2.310299
C	-0.680115	-0.701070	2.533094
H	-0.189618	0.088523	3.108751
H	-1.433920	-1.159326	3.182043
H	0.071478	-1.463256	2.301373
C	-2.482929	-2.369565	0.600097
H	-1.629136	-2.934075	0.988151
H	-3.306579	-2.478026	1.315593
H	-2.794362	-2.840757	-0.336082
C	-3.503289	-0.441813	-1.767037
H	-3.373033	-1.491464	-2.045574
H	-4.553410	-0.301379	-1.487263
H	-3.314469	0.161605	-2.659293
Al	-0.297194	-0.295081	-0.730542
C	1.944985	-0.454940	-0.383114
C	2.841762	-0.793320	-1.406657

C	4.143991	-0.319379	-1.337933
C	4.582377	0.437774	-0.249199
C	3.697830	0.698003	0.794948
C	2.390701	0.224709	0.758374
F	0.910056	-1.636169	0.001170
H	1.709204	0.416251	1.581043
H	4.027345	1.264426	1.661165
H	5.601787	0.805711	-0.211127
H	4.826745	-0.545490	-2.151861
H	2.502978	-1.367900	-2.260064

4h

0 1

Al	-1.283449	-0.638002	0.014774
F	-0.002763	0.042110	1.182737
C	-2.547679	0.864289	-0.009625
C	-3.196557	1.289635	-1.181304
C	-4.111255	2.341228	-1.180722
C	-4.409789	3.001610	0.009773
C	-3.796091	2.595757	1.192280
C	-2.883068	1.540359	1.174690
C	-2.539811	-2.290455	-0.964049
C	-3.068879	-2.112041	0.342014
C	-2.022888	-2.337045	1.275556
C	-0.847241	-2.721183	0.545028
C	-1.171911	-2.686809	-0.843805
C	-3.296065	-2.138885	-2.252652
H	-4.109384	-1.413723	-2.152930
H	-3.738907	-3.091724	-2.565670
H	-2.643457	-1.801151	-3.064513
C	-4.466091	-1.665415	0.653734
H	-4.797163	-0.882133	-0.035879
H	-4.538295	-1.254761	1.664282
H	-5.169320	-2.502717	0.580316
C	-2.104140	-2.260669	2.774066
H	-2.936792	-1.631168	3.099651
H	-1.185661	-1.843706	3.199134
H	-2.248104	-3.254401	3.213806
C	0.425924	-3.204514	1.176700
H	1.241515	-3.279637	0.453451
H	0.269779	-4.194934	1.620637
H	0.762873	-2.532132	1.971185
C	-0.270928	-3.049233	-1.988350
H	-0.564343	-4.014480	-2.416254
H	0.769639	-3.122554	-1.664898
H	-0.315601	-2.303572	-2.788739
Al	1.283454	0.637990	-0.014765
F	0.002774	-0.042137	-1.182728
C	2.547703	-0.864285	0.009624
C	3.196592	-1.289623	1.181300
C	4.111312	-2.341197	1.180710
C	4.409859	-3.001564	-0.009789
C	3.796155	-2.595714	-1.192294
C	2.883111	-1.540335	-1.174696
C	2.539791	2.290456	0.964049
C	3.068855	2.112053	-0.342018
C	2.022856	2.337045	-1.275554
C	0.847205	2.721160	-0.545018
C	1.171886	2.686796	0.843811
C	3.296057	2.138899	2.252645
H	4.109374	1.413733	2.152924
H	3.738904	3.091740	2.565648
H	2.643457	1.801175	3.064516
C	4.466073	1.665449	-0.653745
H	4.797160	0.882173	0.035866
H	4.538278	1.254796	-1.664293
H	5.169288	2.502762	-0.580331
C	2.104099	2.260666	-2.774064
H	2.936762	1.631182	-3.099652
H	1.185626	1.843681	-3.199124
H	2.248039	3.254400	-3.213809
C	-0.425981	3.204448	-1.176684
H	-1.241568	3.279549	-0.453427
H	-0.269871	4.194869	-1.620630
H	-0.762917	2.532047	-1.971159
C	0.270897	3.049192	1.988361
H	0.564302	4.014433	2.416285
H	-0.769670	3.122509	1.664907
H	0.315574	2.303516	2.788736
H	4.587287	-2.650920	2.107200
H	2.970709	-0.801946	2.129721
H	2.411582	-1.246560	-2.112901
H	4.027691	-3.101393	-2.126046
H	5.118890	-3.824285	-0.015848
H	-2.970682	0.801948	-2.129723
H	-4.587223	2.650956	-2.107214
H	-5.118803	3.824346	0.015826
H	-4.027616	3.101448	2.126028
H	-2.411544	1.246583	2.112896

4h'

0 1

Al	-1.432902	-0.394927	-0.037686
F	-0.020374	-0.631530	1.172092
C	-1.646028	1.550797	0.032016
C	-1.361062	2.394252	-1.053135
C	-1.489406	3.778917	-0.961634
C	-1.910755	4.361771	0.230979
C	-2.201700	3.552831	1.326437
C	-2.071066	2.169828	1.218885
C	-3.421340	-0.959208	-1.118007
C	-3.782087	-0.637010	0.215221
C	-3.046083	-1.476806	1.088508
C	-2.267566	-2.378257	0.283936
C	-2.508564	-2.053397	-1.087689
C	-3.910915	-0.233947	-2.338120
H	-3.753019	0.847214	-2.244771
H	-4.983123	-0.398139	-2.494546
H	-3.386461	-0.570345	-3.236912
C	-4.744530	0.451258	0.582473
H	-4.510611	1.383443	0.057674
H	-4.727193	0.665454	1.654150
H	-5.767405	0.159868	0.316721
C	-3.101117	-1.526629	2.589374
H	-3.525282	-0.609186	3.006030
H	-2.102255	-1.657294	3.019216
H	-3.720236	-2.363215	2.934589
C	-1.477033	-3.527388	0.841521
H	-1.197537	-4.233526	0.056177
H	-2.073039	-4.072185	1.581704
H	-0.557972	-3.197281	1.337498
C	-1.952400	-2.752925	-2.297386
H	-2.740431	-2.907335	-3.040545
H	-1.555986	-3.736976	-2.032901
H	-1.145998	-2.187273	-2.776355
Al	1.432849	-0.394609	0.037565
F	0.020372	-0.631374	-1.172205
C	1.646017	1.551077	-0.031759
C	2.070850	2.170158	-1.218638
C	2.200548	3.553260	-1.326476
C	1.908793	4.362182	-0.231277
C	1.487622	3.779257	0.961411
C	1.360219	2.394562	1.053192
C	3.044976	-1.478007	-1.088539
C	3.782391	-0.636988	-0.217622
C	3.423632	-0.957078	1.116618
C	2.510377	-2.050875	1.089401
C	2.267379	-2.377963	-0.281400
C	3.098107	-1.530391	-2.589382
H	3.519912	-0.612870	-3.008283
H	3.718348	-2.366404	-2.933972
H	2.098890	-1.663708	-3.017564
C	4.744591	0.450445	-0.587969
H	4.725693	0.663036	-1.659946
H	4.511791	1.383464	-0.064148
H	5.767797	0.159134	-0.323396
C	3.914814	-0.229446	2.334664
H	3.752378	0.851085	2.241544
H	3.395091	-0.567626	3.235524
H	4.988239	-0.389362	2.487063
C	1.954997	-2.748062	2.300822
H	1.557692	-3.732294	2.038341
H	2.743624	-2.901783	3.043491
H	1.149375	-2.181164	2.779612
C	1.476261	-3.528173	-0.835898
H	2.071664	-4.074763	-1.575253
H	1.197119	-4.232489	-0.048805
H	0.556967	-3.199014	-1.332018
H	2.305752	1.558312	-2.091146
H	2.525057	4.000043	-2.262579
H	2.001358	5.441843	-0.308702
H	1.241750	4.404731	1.815184
H	-2.305388	1.557982	2.091548
H	-2.526316	3.999656	2.262488

H	-2.004186	5.441365	0.308300
H	-1.244137	4.404316	-1.815637
H	0.996033	1.967678	1.986797
H	-0.996779	1.967455	-1.986749

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